



New developments in the McStas neutron instrument simulation package

Willendrup, Peter Kjær; Bergbäck Knudsen, Erik; Klinkby, Esben Bryndt; R. Nielsen, Torben; Farhi, E.; Filges, U.; Lefmann, K.

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New developments in the McStas neutron instrument simulation package

Peter Willendrup^{1,2}, Erik Knudsen¹, Esben Klinkby^{3,4},
Torben R Nielsen², E Farhi⁵, U Filges⁶, K Lefmann⁷

¹NEXMAP, Physics Department, Technical University of Denmark, Denmark

²ESS Data Management & Software Center, Denmark

³Center for Nuclear Technologies, Technical University of Denmark, Denmark

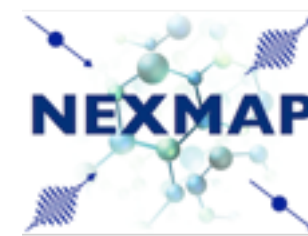
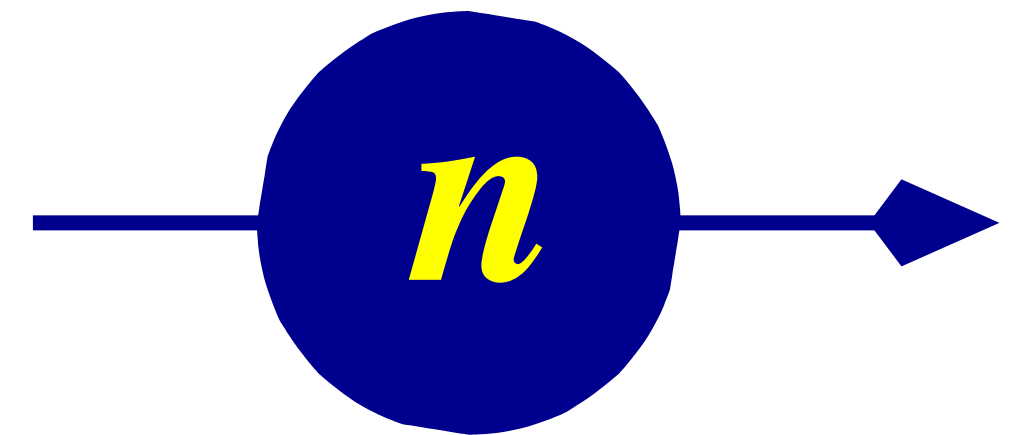
⁴ESS Neutronics Group, Sweden

⁵CS-group, Institut Laue-Langevin (ILL), France

⁶LDM, Paul Scherrer Institute (PSI), Switzerland

⁷eScience and Nano-Science centers, Niels Bohr Institute (NBI), Denmark

McStas



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Agenda

- A brief introduction to McStas, Monte Carlo & raytracing
- Highlighted new features in McStas 2.1
 - McStas-MCNP for background estimates
 - McStas-Mantid event processing
 - Speedup in Single_crystal.comp

McStas Introduction

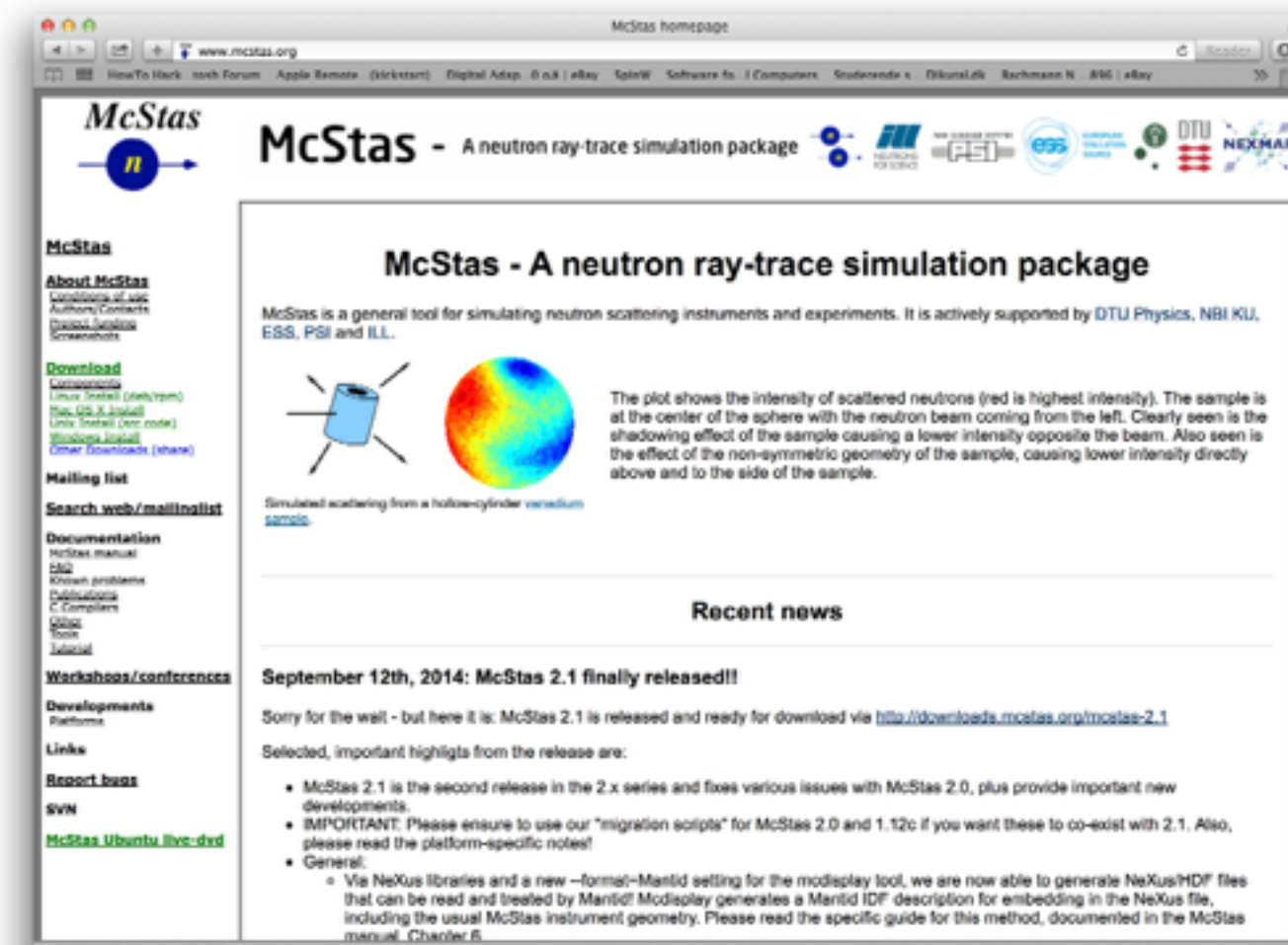
- Flexible, general simulation utility for neutron scattering experiments.
- Original design for Monte carlo Simulation of triple axis spectrometers
- Developed at DTU Physics, ILL, PSI, Uni CPH, **ESS**
- V. 1.0 by K Nielsen & K Lefmann (1998) RISØ
- Currently 2.5+1 people full time plus students



GNU GPL
license
Open Source

Project website at
<http://www.mcstas.org>

mcstas-users@mcstas.org mailinglist



McXtrace homepage - Mozilla Firefox

File Edit View History Bookmarks Tools Help

McXtrace homepage

www.mcxtrace.org

Google

Most Visited Getting Started A/B Trøjborg 1 Latest Headlines latex-lab projec... publications.li Viewing Feed McCode: {8} A... Import to Mendeley

McXtrace

McXtrace - An X-ray ray-trace simulation package

ESRF SAXS LAB GANESHA DTU

McXtrace - Monte Carlo Xray Tracing, is a joint venture by

DTU ESRF SAXS LAB

This site is undergoing reorganization. Inconsistencies and broken links may occur. Please do report any findings to erkn_AT_fysik.dtu.dk if you have the time. Thanks in advance.

Funding from NABIIT, [DSF](#) and the above parties.

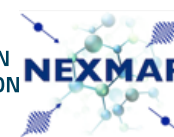
McStas

[McXtrace](#)
[Project Status](#)
[Project Partners](#)
[Project People](#)
[Goal](#)
[Mailing List](#)
[Links](#)
[Publications](#)
[Minutes of Meetings](#)
[McXtrace Art](#)
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New developments in McStas



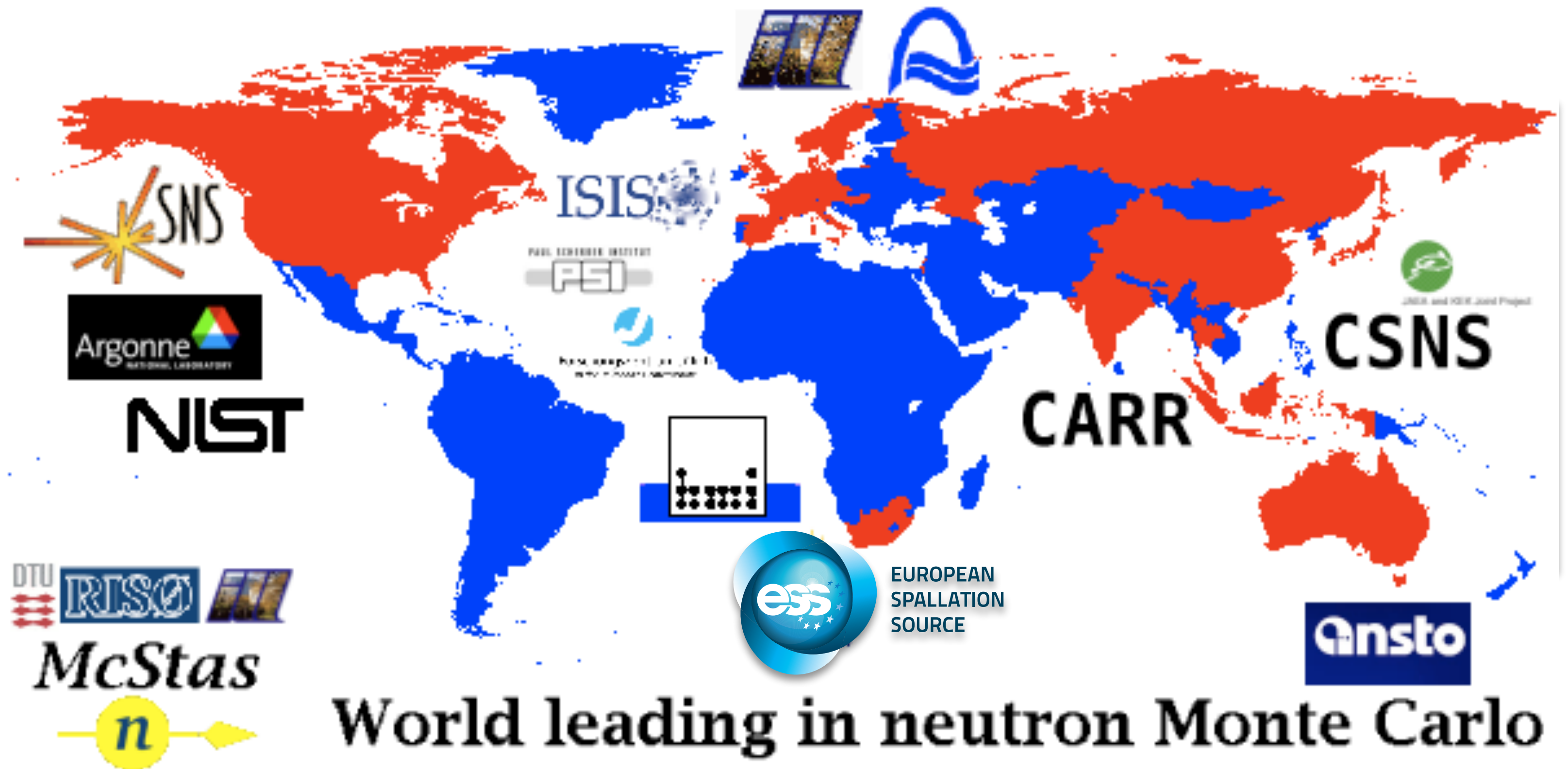
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PAUL SCHERRER INSTITUT
PSI



McStas Introduction

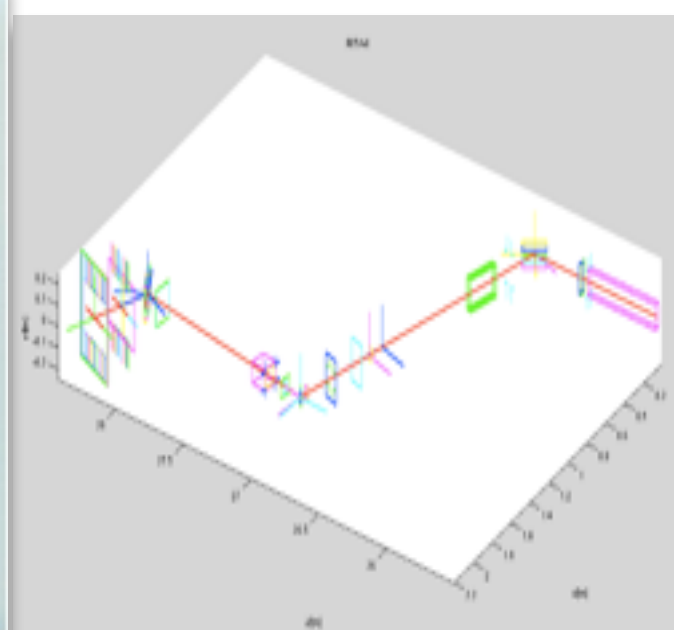
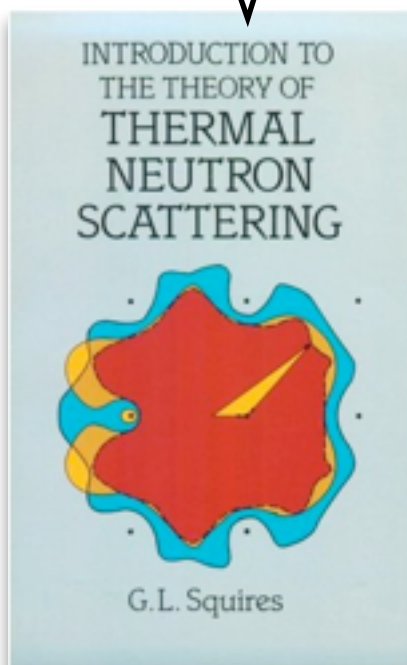
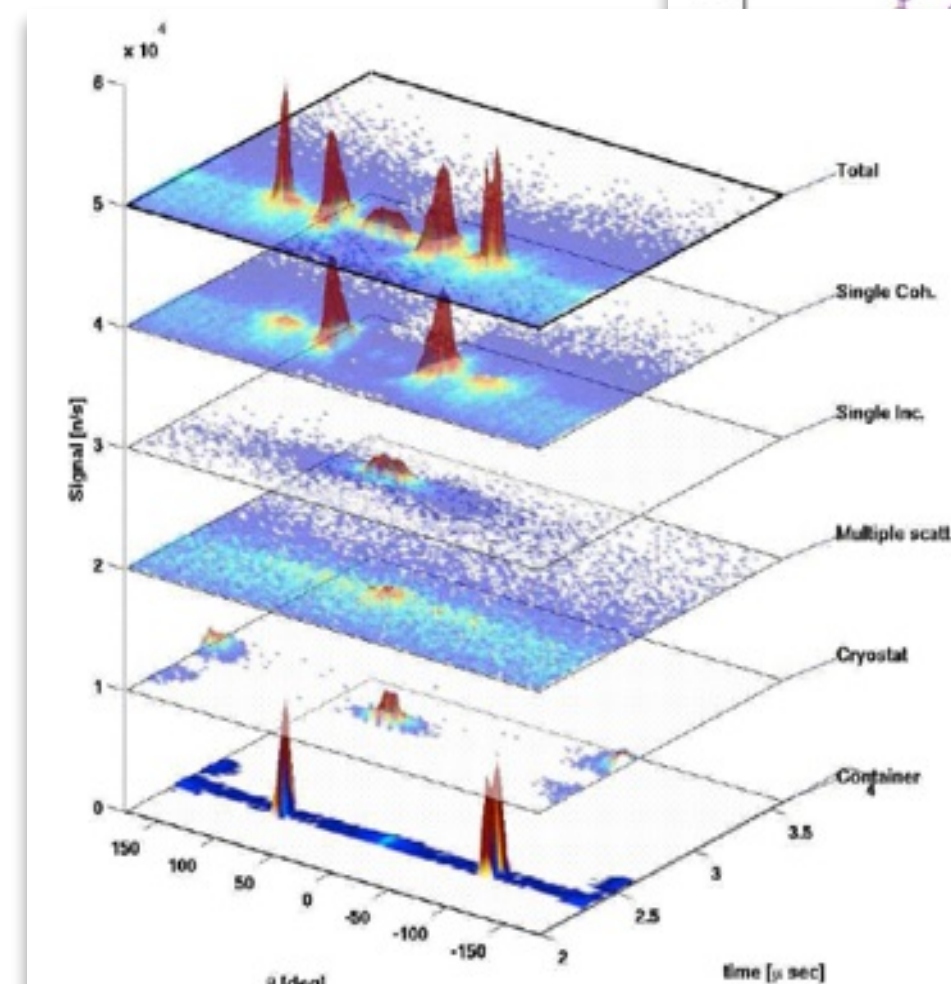
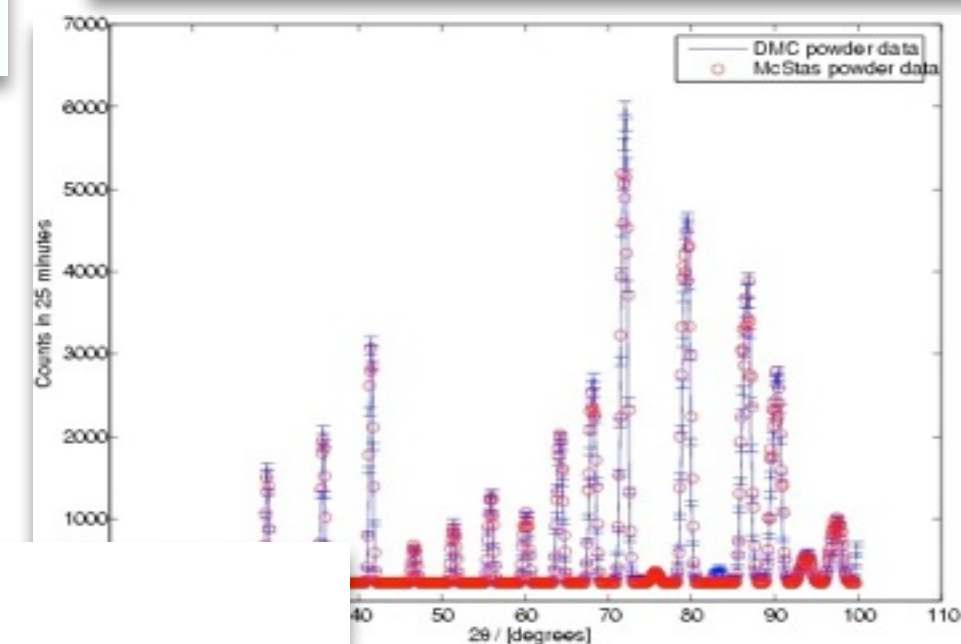
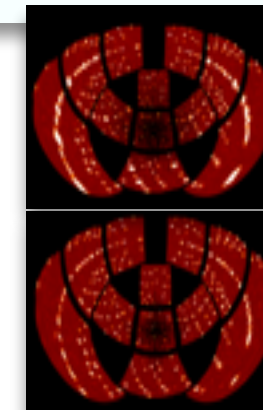
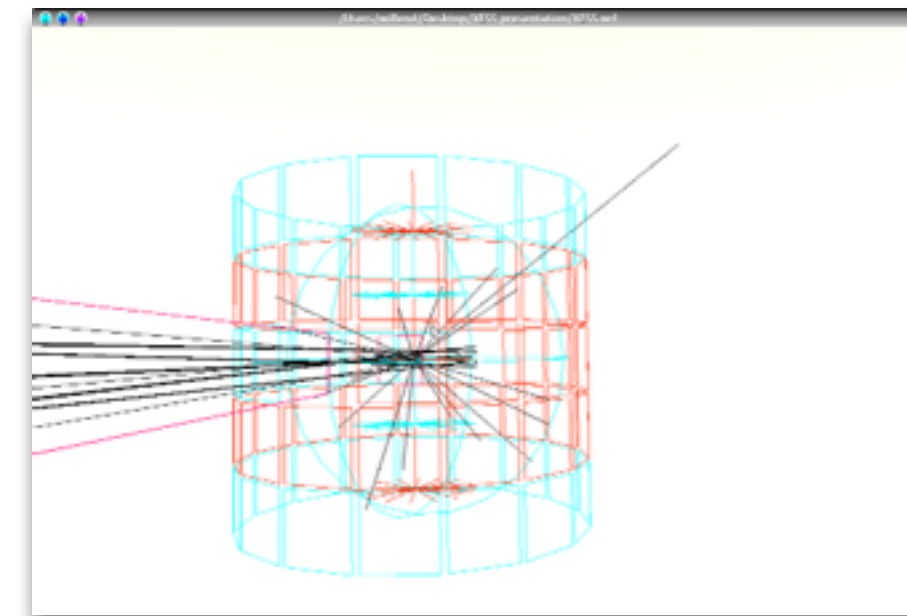
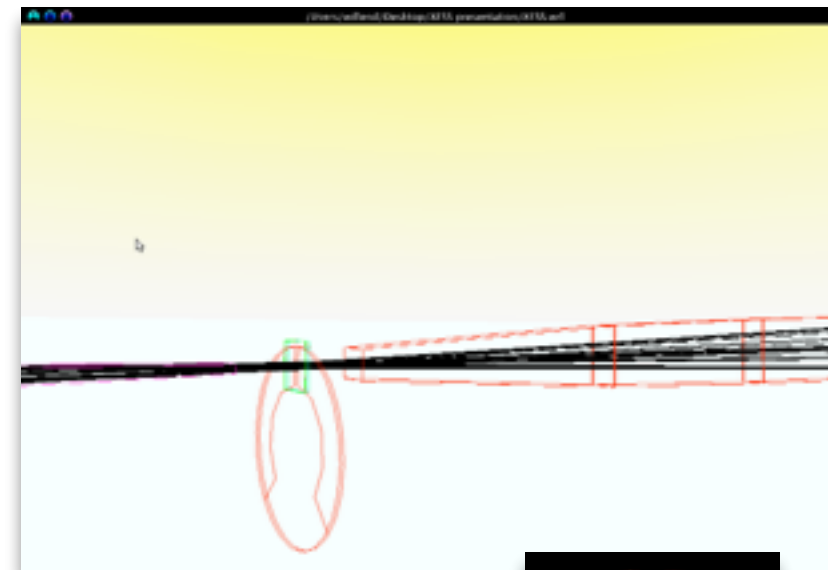


New developments in McStas

What is McStas used for?

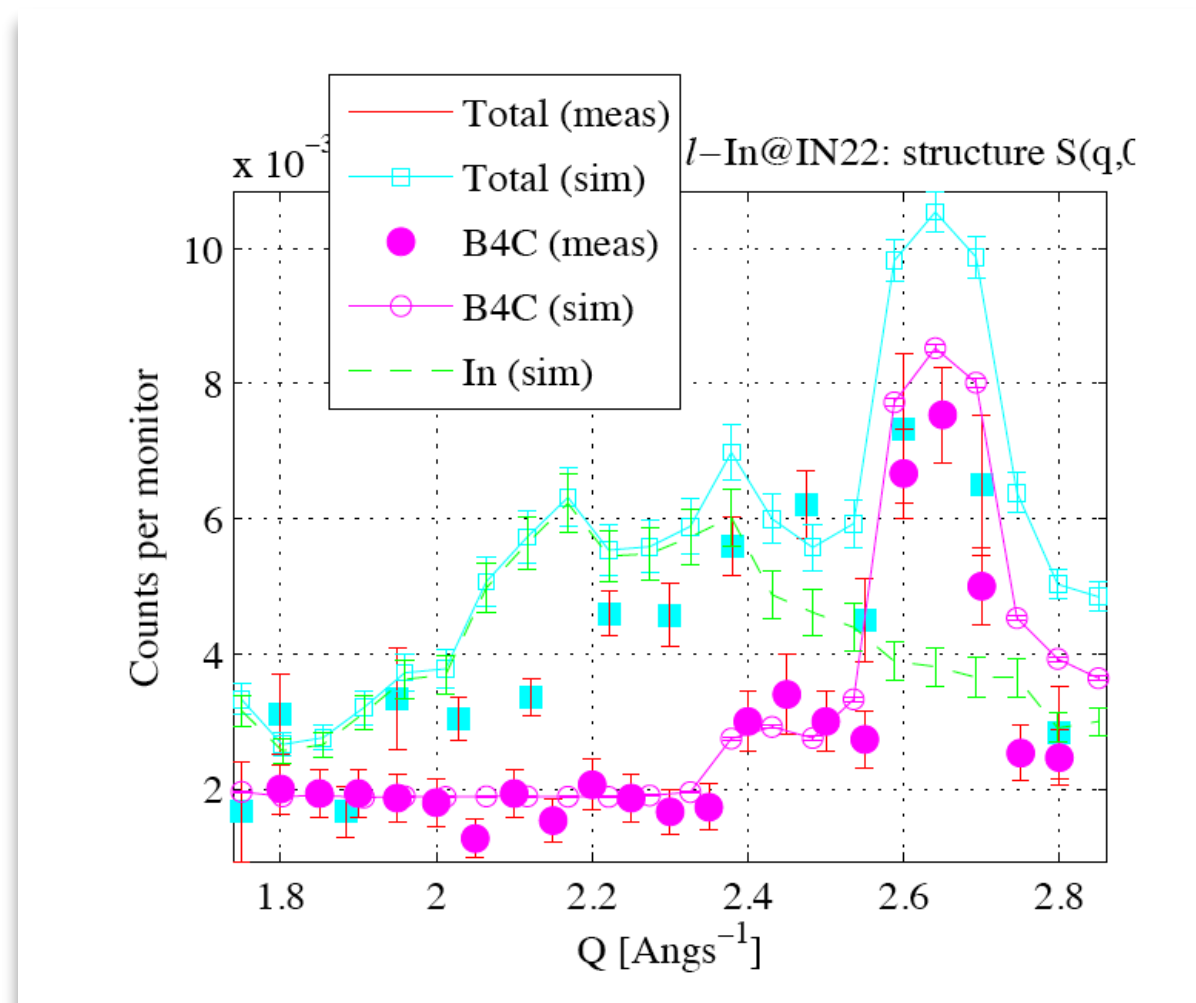
- Instrumentation
- Virtual experiments
- Data analysis
- Teaching

(KU, DTU)

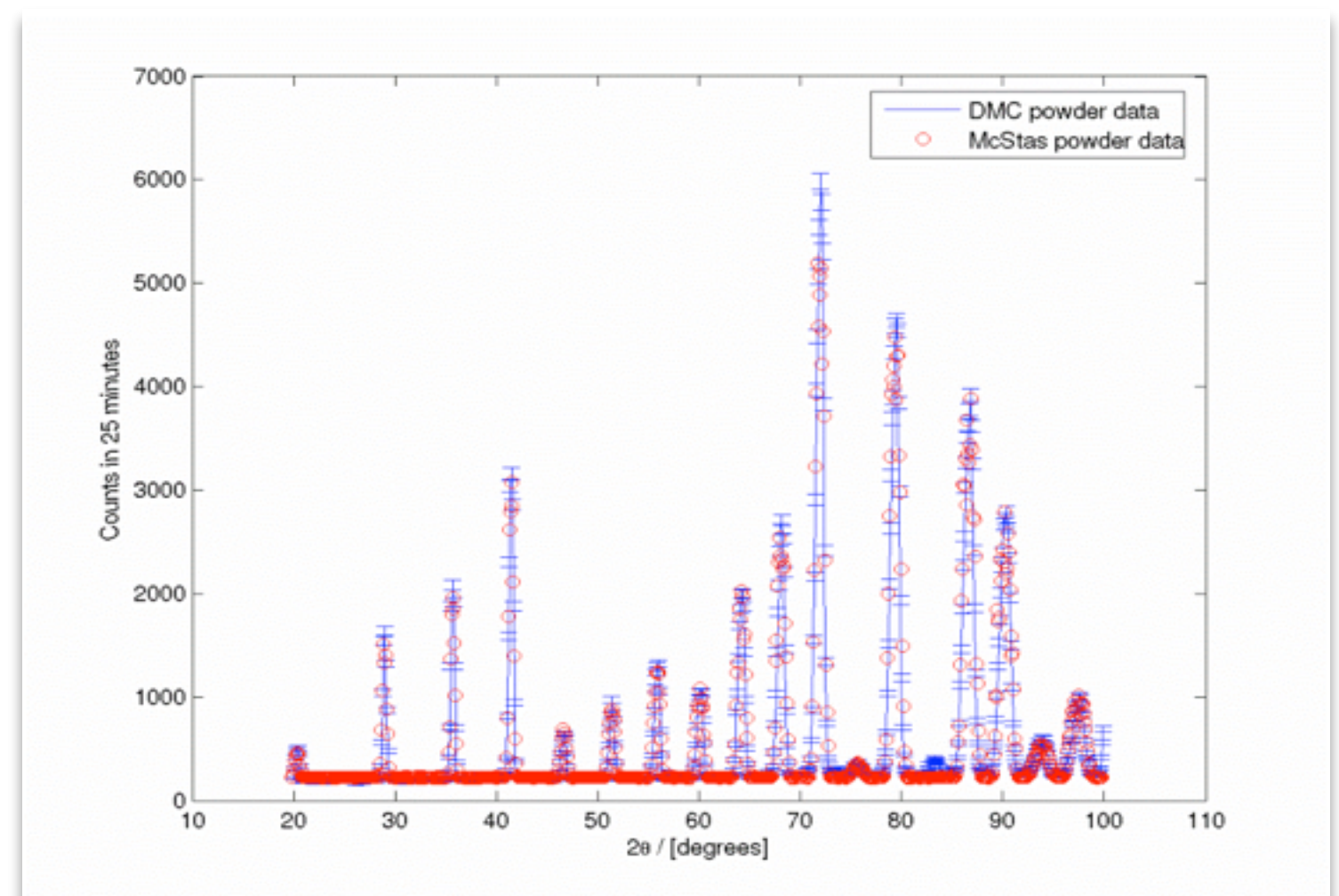


Reliability - cross comparisons

- Much effort has gone into this
- Here: simulations vs. exp. at powder diffract. DMC, PSI
- The bottom line is
- McStas agrees very well with other packages (NISP, Vitess, IDEAS, RESTRAX, ...)
- Experimental line shapes are within 5%
- Absolute intensities are within 10%
- Common understanding: McStas and similar codes are reliable



E. Farhi, P. Willendrup et al., in preparation



P. Willendrup et al., Physica B, 386, (2006), 1032.

Neutron ray/package:

Weight (p): # neutrons (left) in the package

Coordinates (x,y,z)

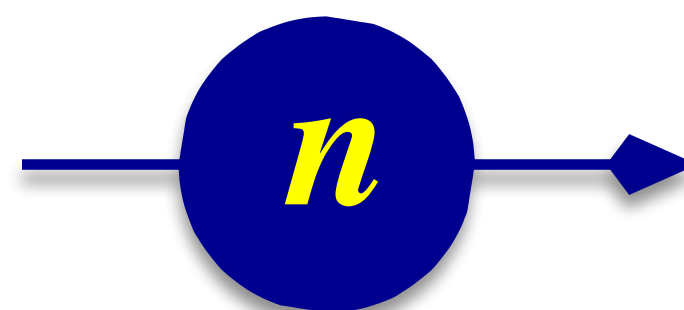
Velocity (v_x, v_y, v_z)

Spin (s_x, s_y, s_z)

Time (t)

Instrument: positioning + transformation between sequential component coordinate systems, e.g. neutron source, crystal, detector.

McStas



Monochromatic neutron source

Detector

θ

x'

y'

θ

z'

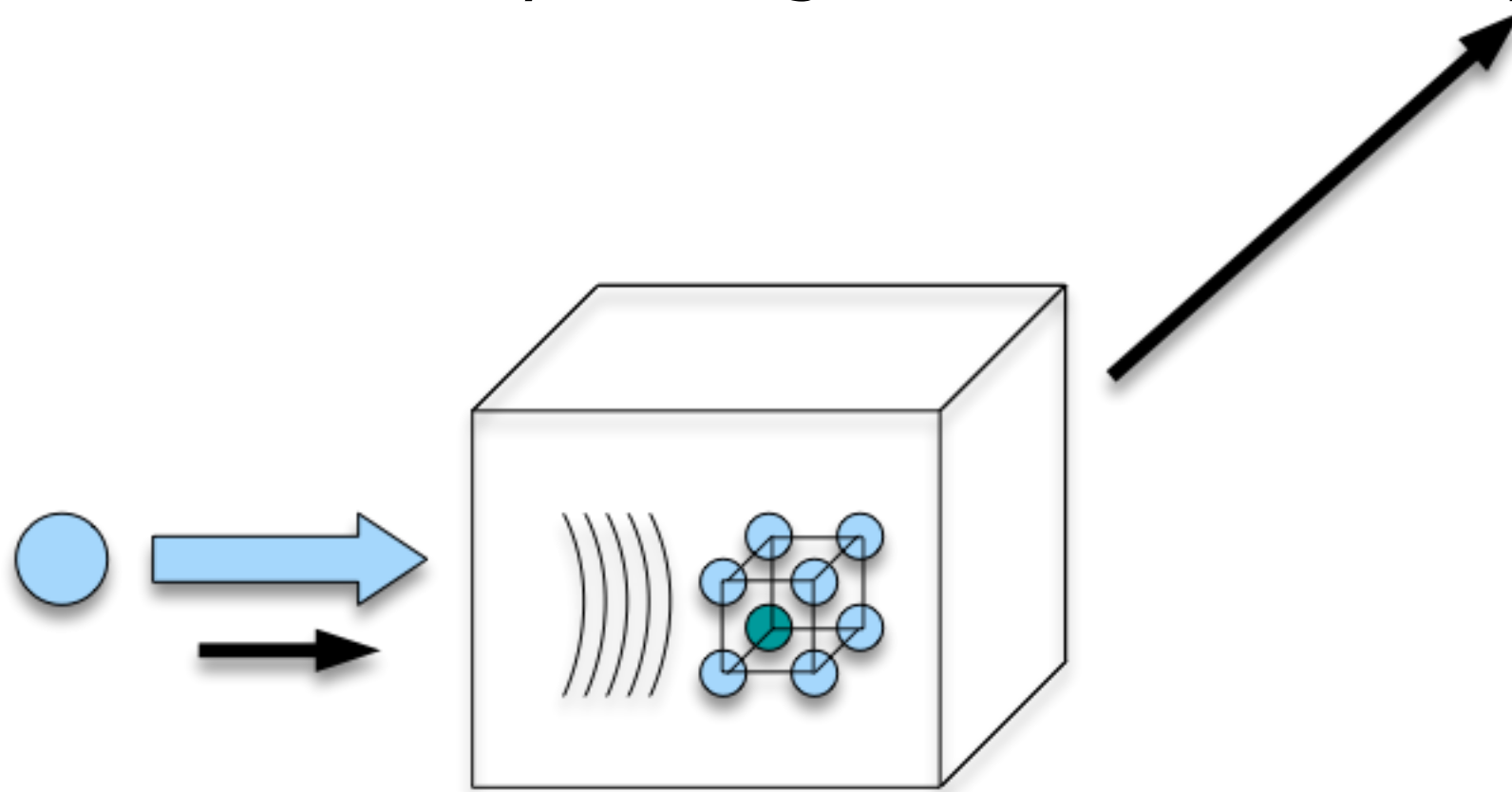
Components: Here the neutron physics happen, neutron weight adjusted according to scattering probabilities etc.

Local, internal coordinate system!

Bragg scattering condition

Elements of Monte-Carlo raytracing

- Instrument Monte Carlo methods implement coherent scattering effects
- Uses deterministic propagation where this can be done
- Uses Monte Carlo sampling of “complicated” distributions and stochastic processes and multiple outcomes with known probabilities are involved
- - I.e. inside scattering matter
- Uses the particle-wave duality of the neutron to switch back and forward between deterministic ray tracing and Monte Carlo approach



- Result: A realistic and efficient transport of neutrons in the thermal and cold range

McStas overview

- Portable code (Unix/Linux/Mac/Windows)

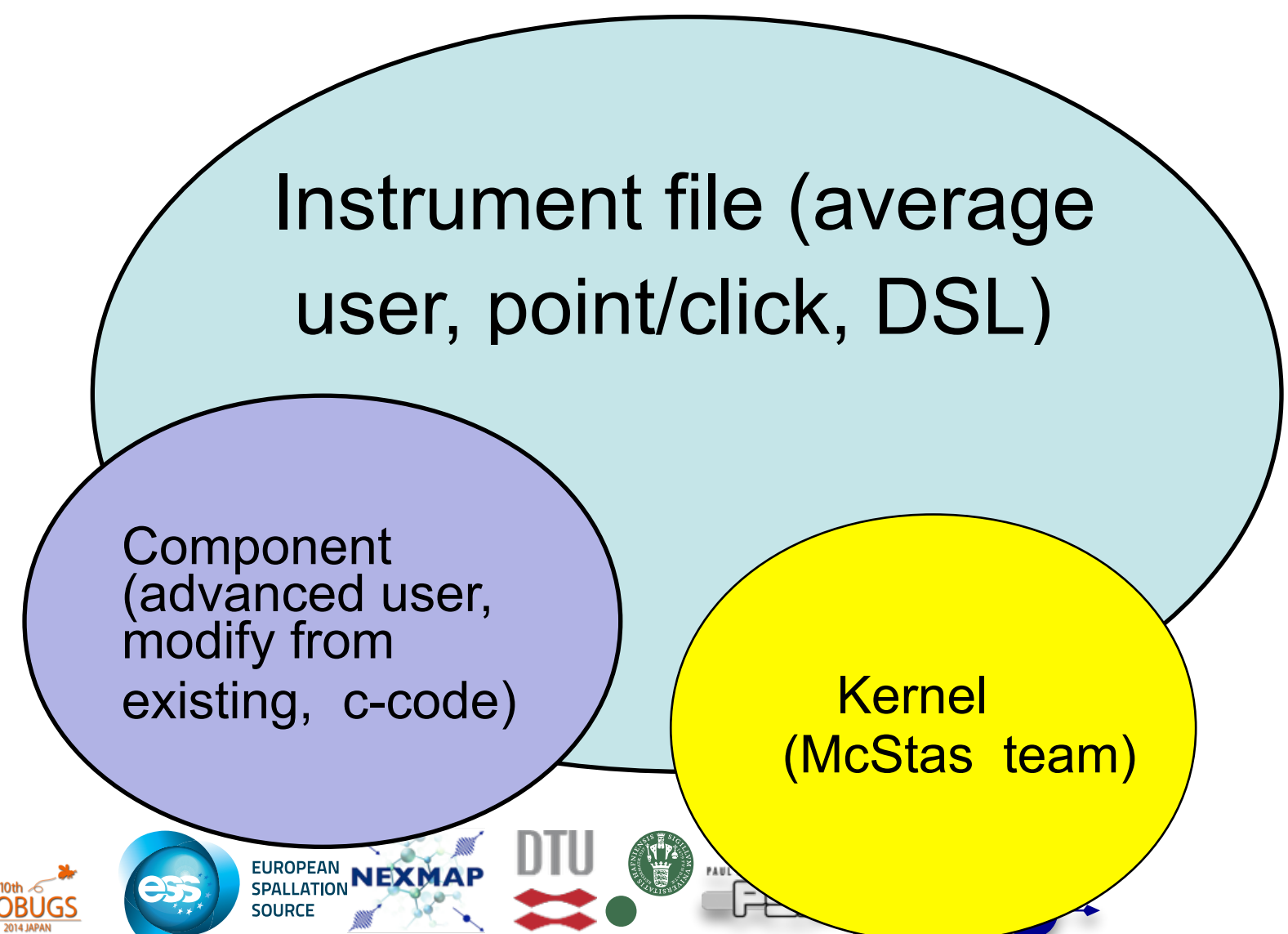
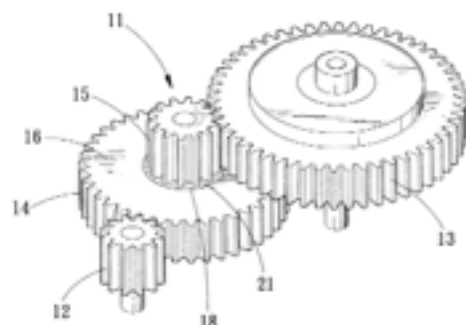


- Ran on everything from iPhone to 1000+ node cluster!

- 'Component' files (~150) inserted from library

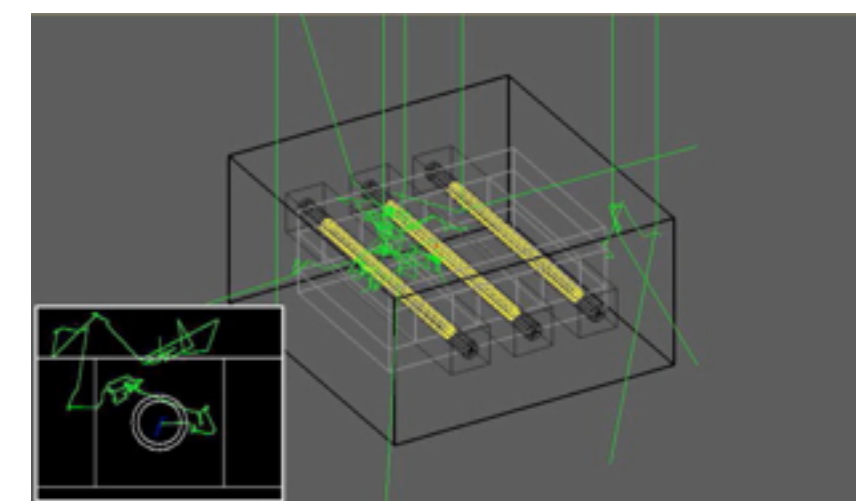
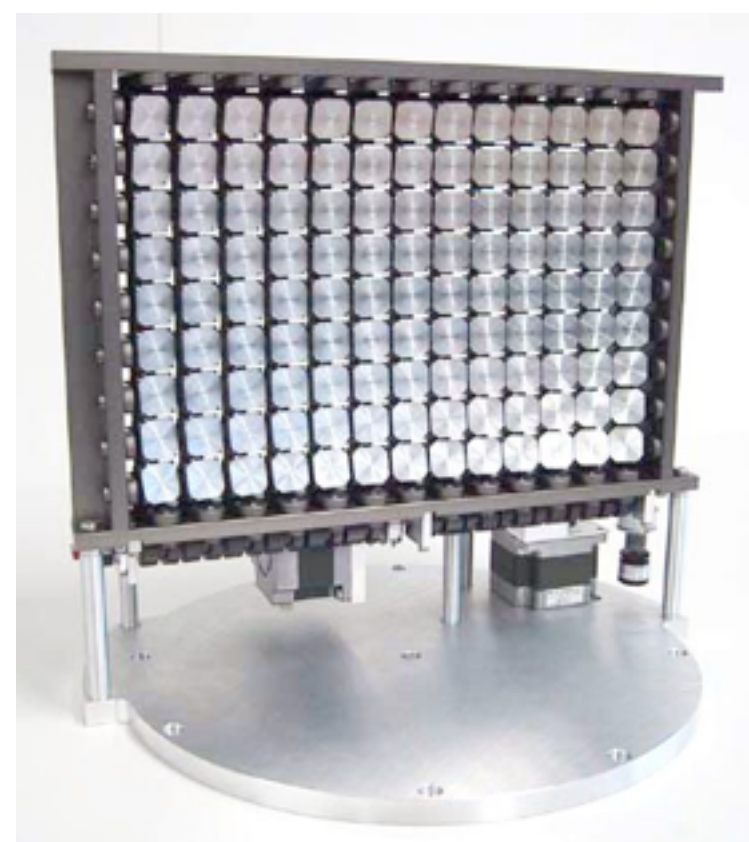
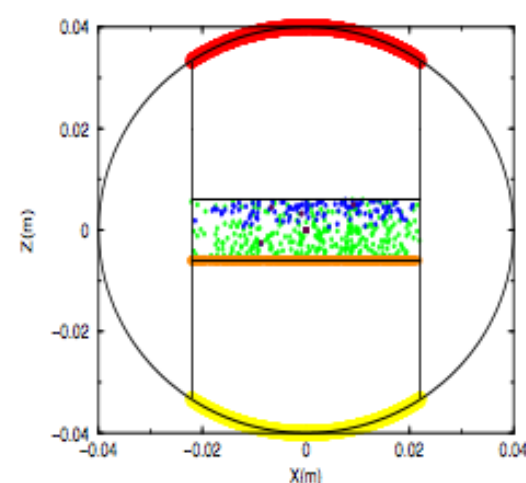
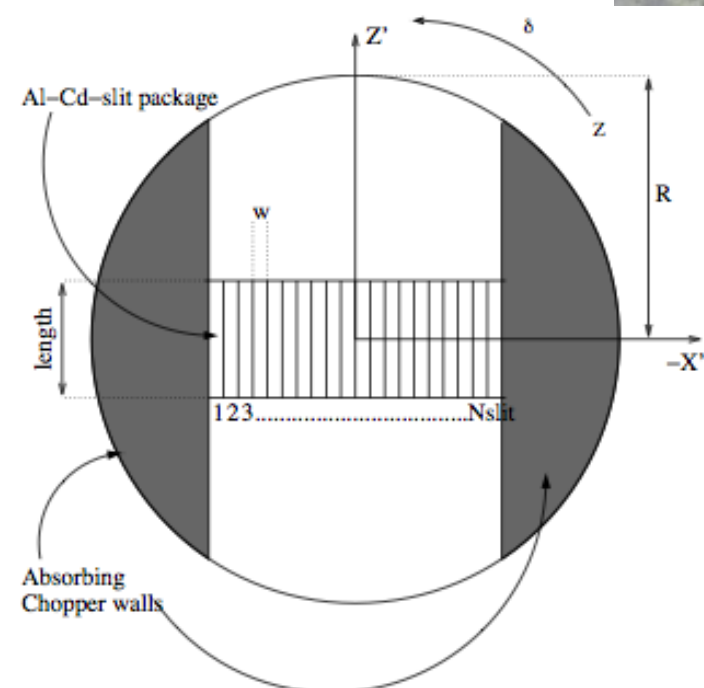
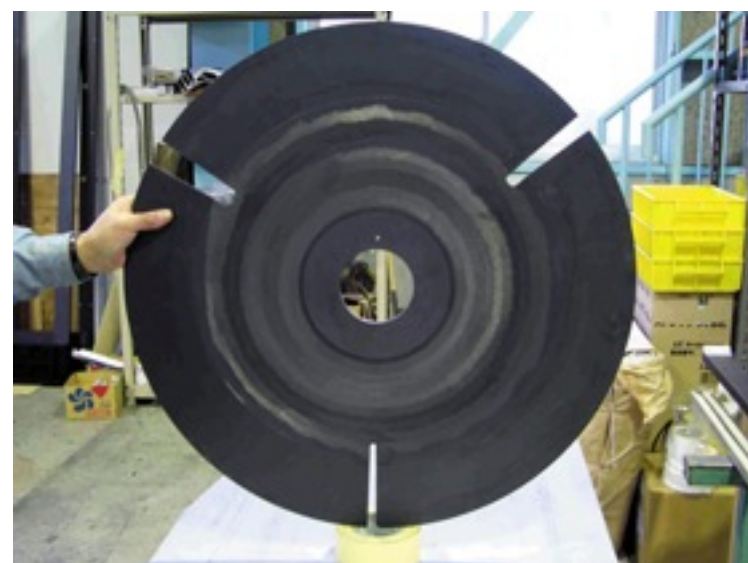
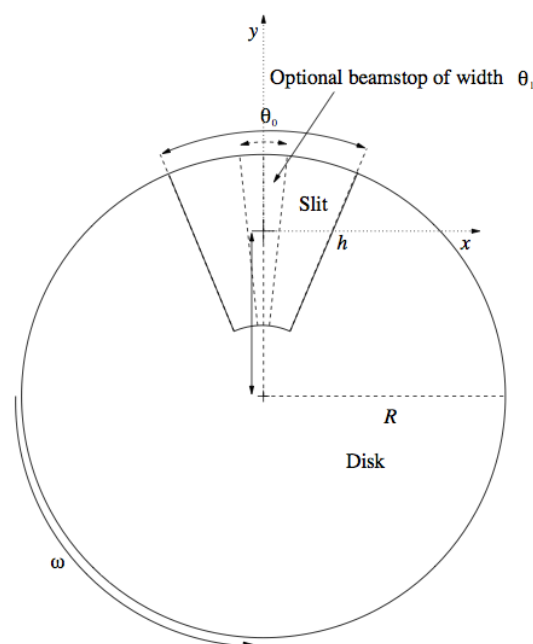
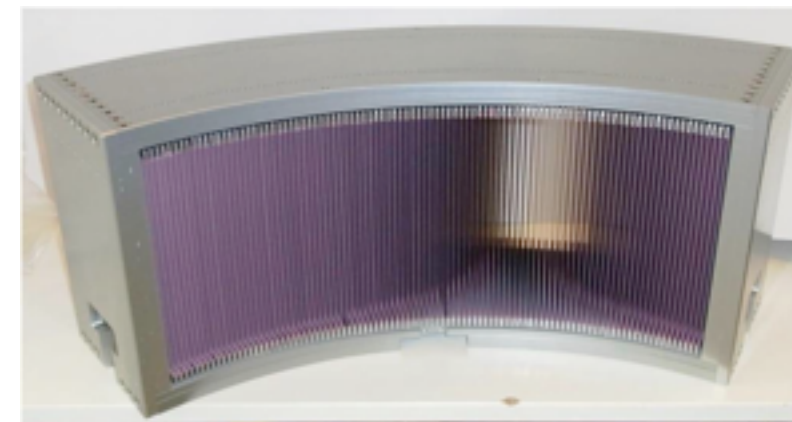
- Sources
- Optics
- Samples
- Monitors
- If needed, write your own comps

- DSL + ISO-C code gen.



New developments in McStas

Neutron optics and other instrument components

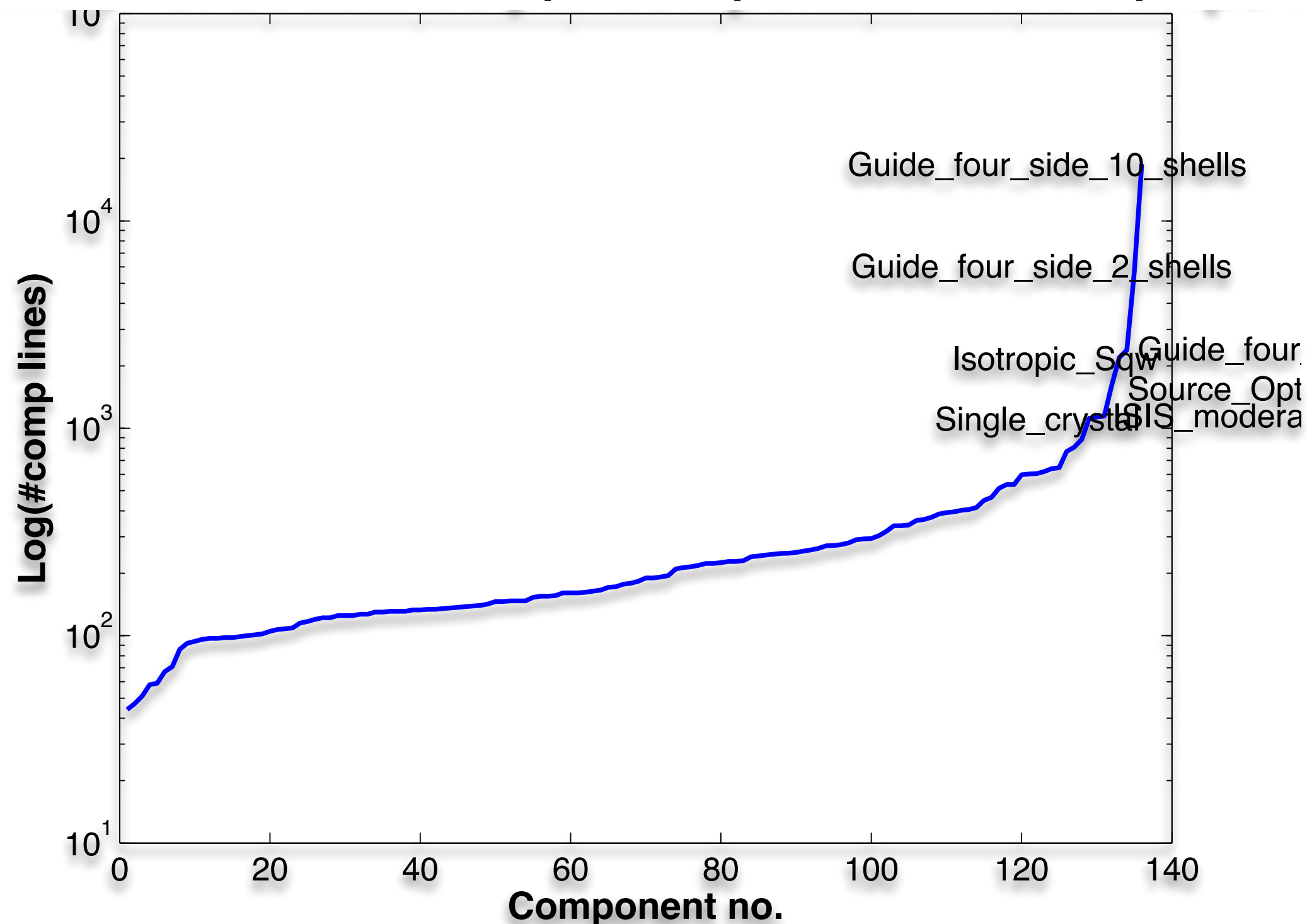


New developments in McStas

Writing new comps or understanding existing is not that complex...

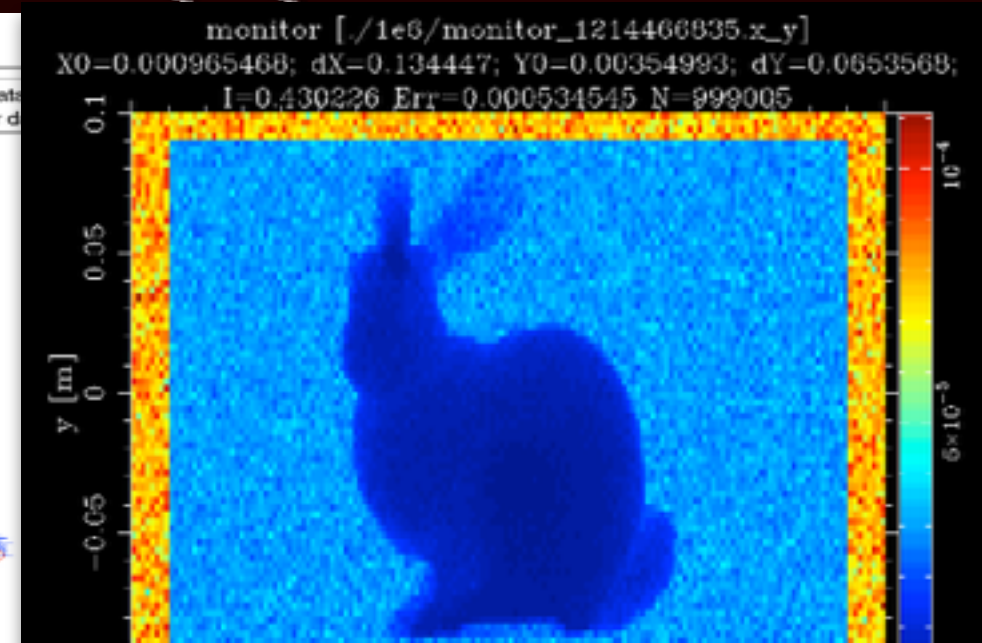
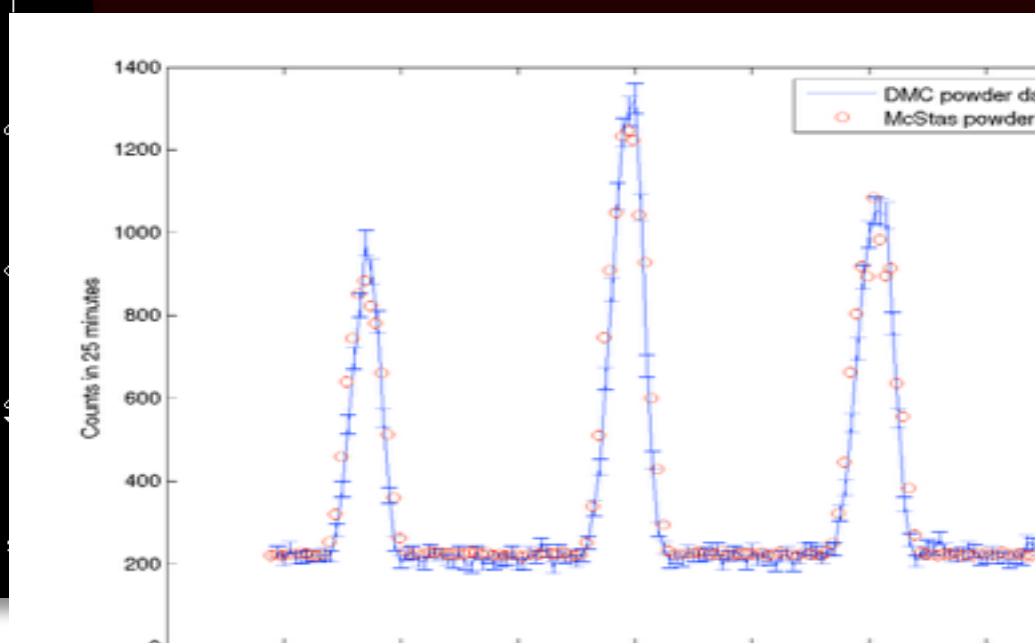
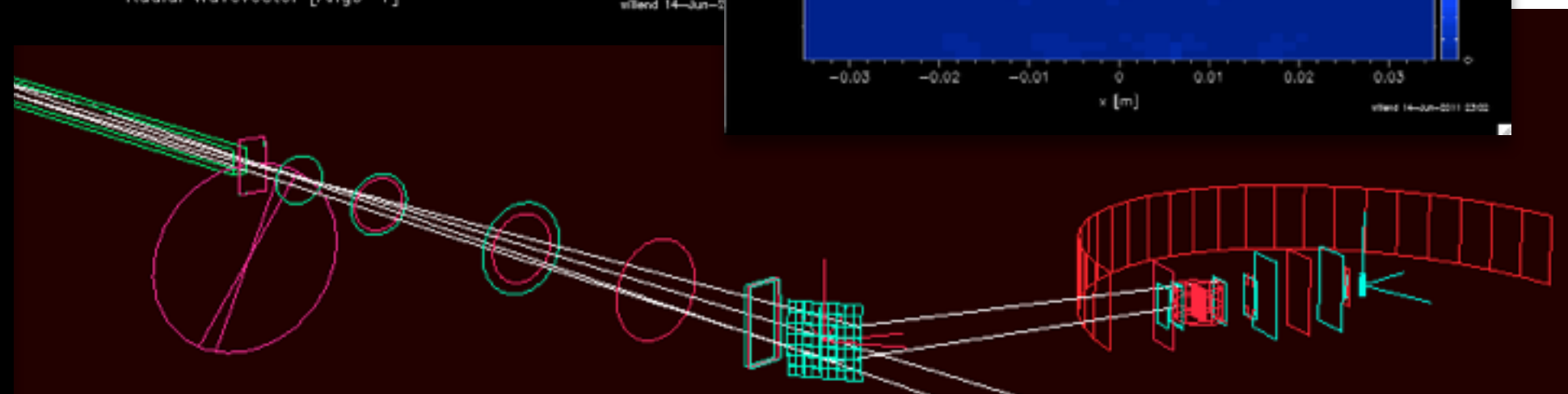
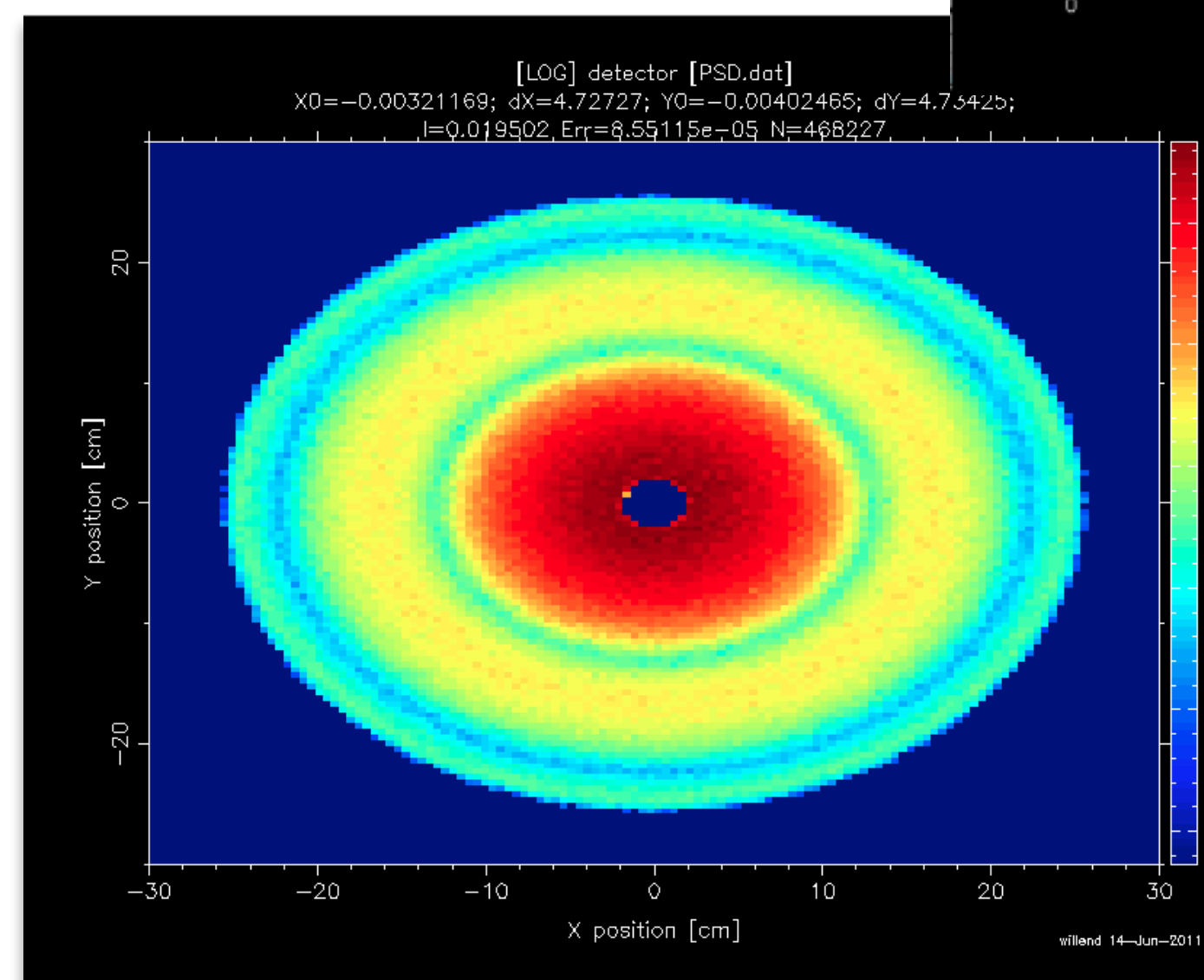
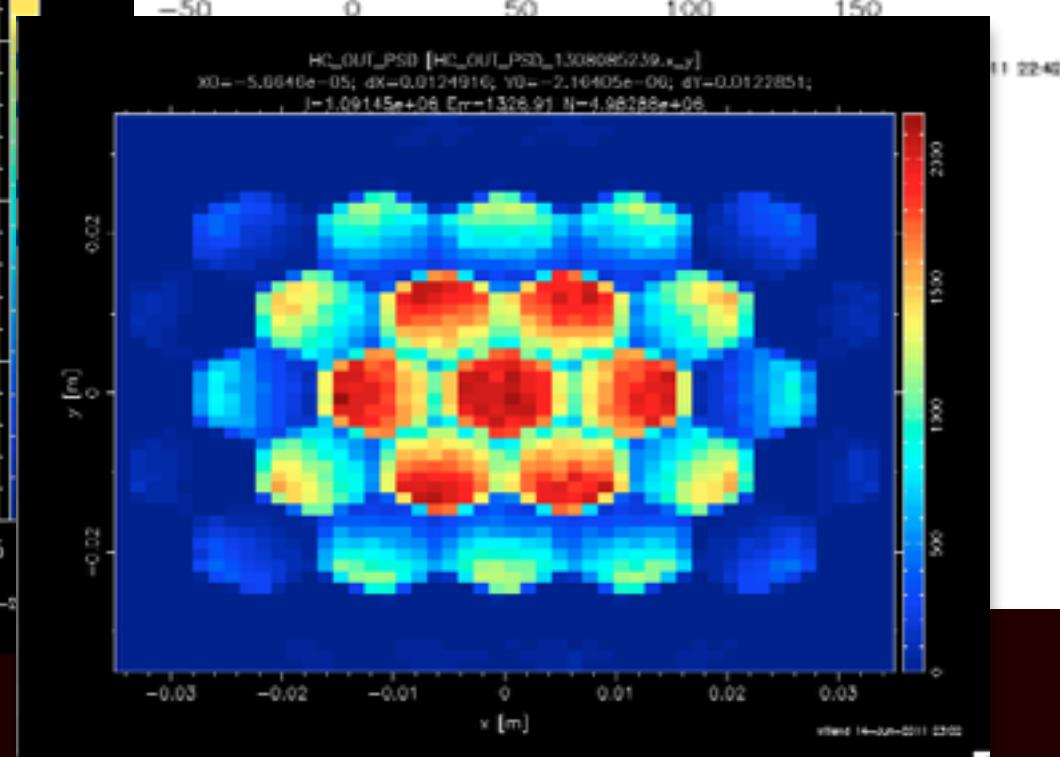
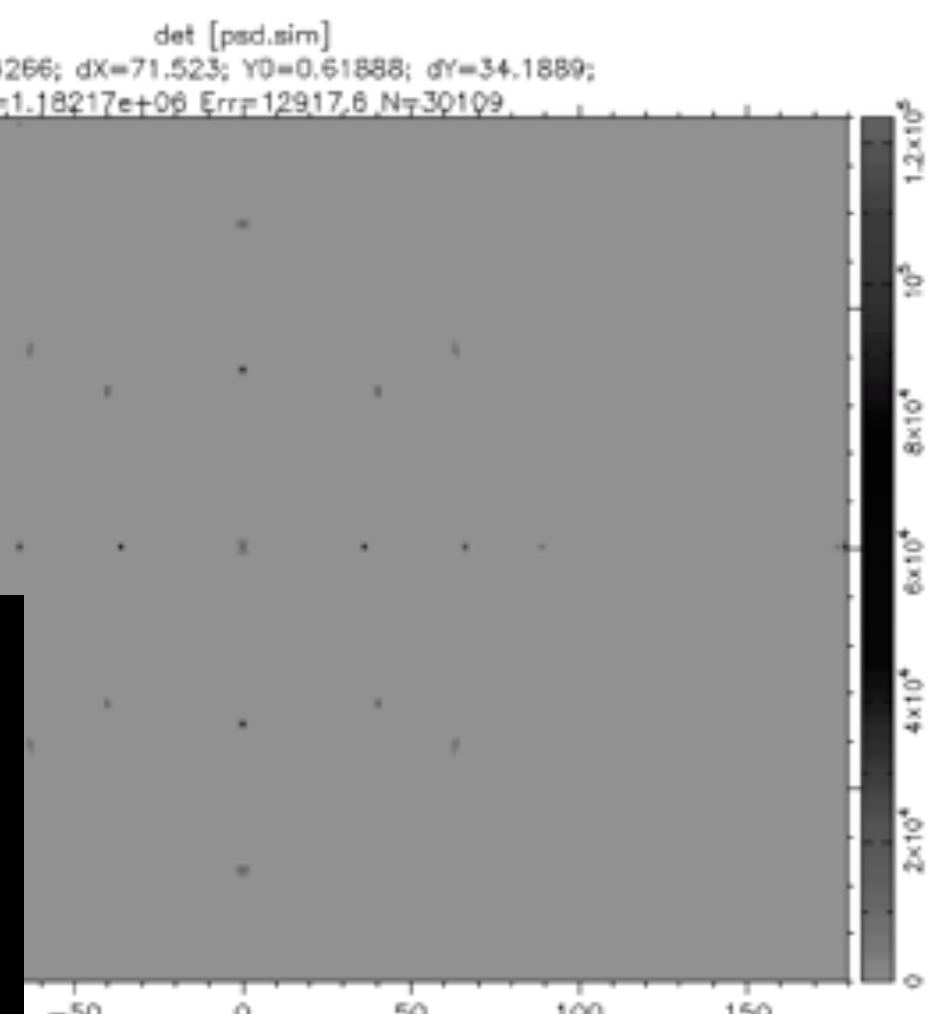
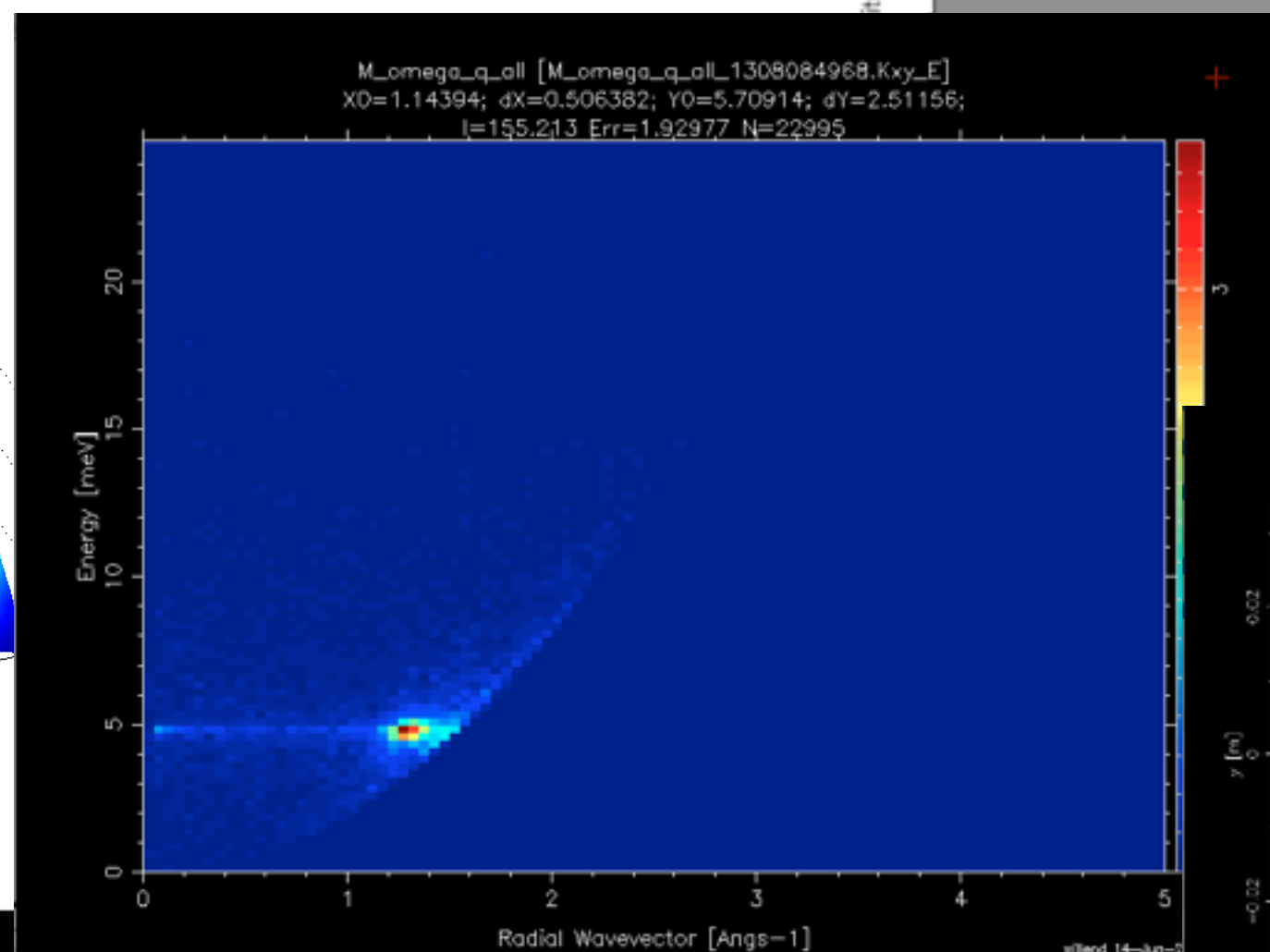
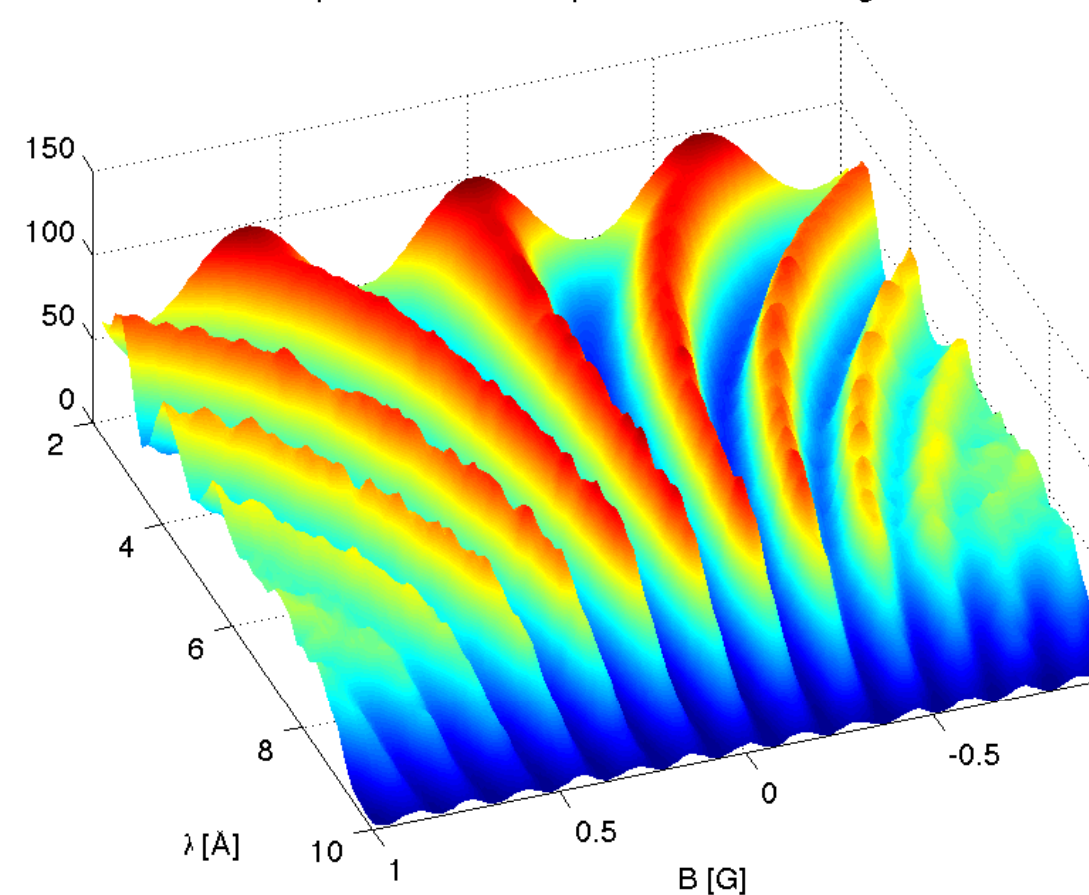
- Check our long list of components and look inside... Most of them are quite simple and short... Statistics:

Number of lines of code per component - 165 comps in total



Example suite: 123 instruments

Spin-echo B scan dependence of wavelength



McStas-MCNPX interfaces for beam losses

1 m

1 m

5 cm

$$\mathbf{n}_t = (\mathbf{r}_t, \mathbf{v}_t, t_t, \mathbf{s}_t, p_i - p_r)$$

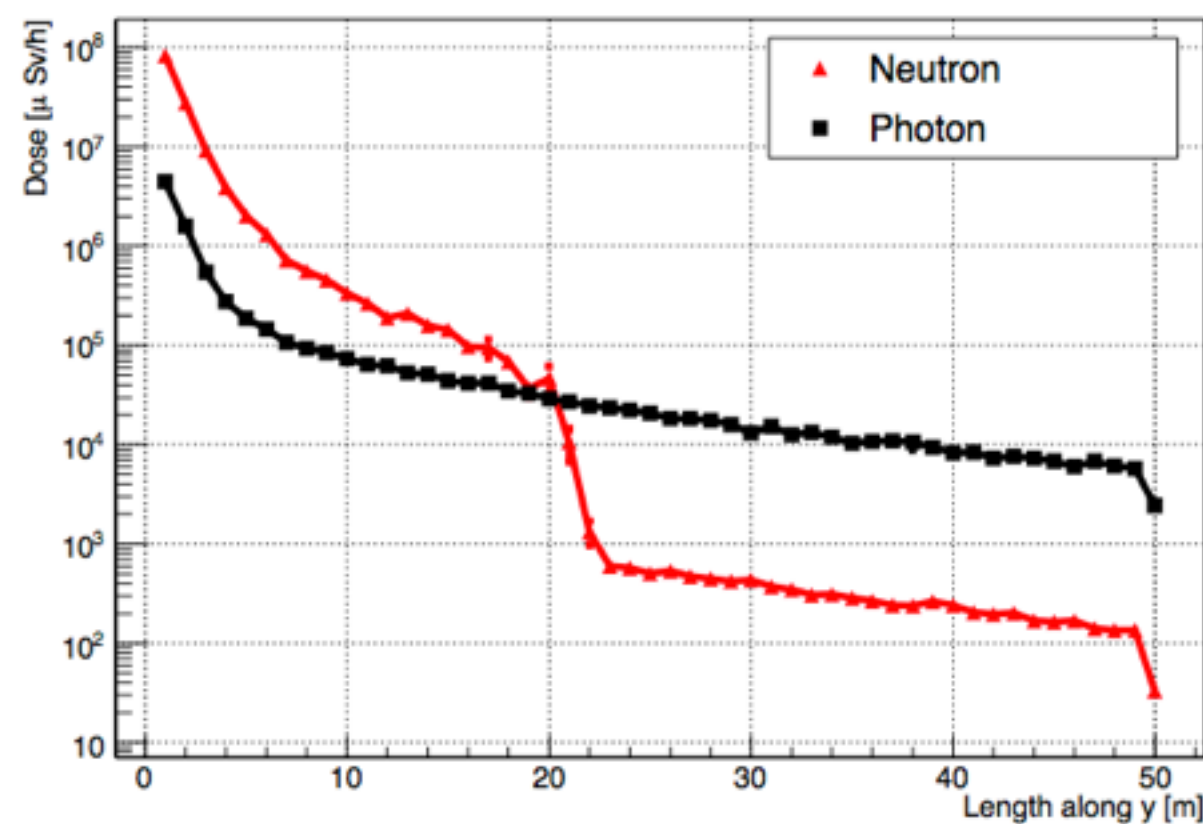
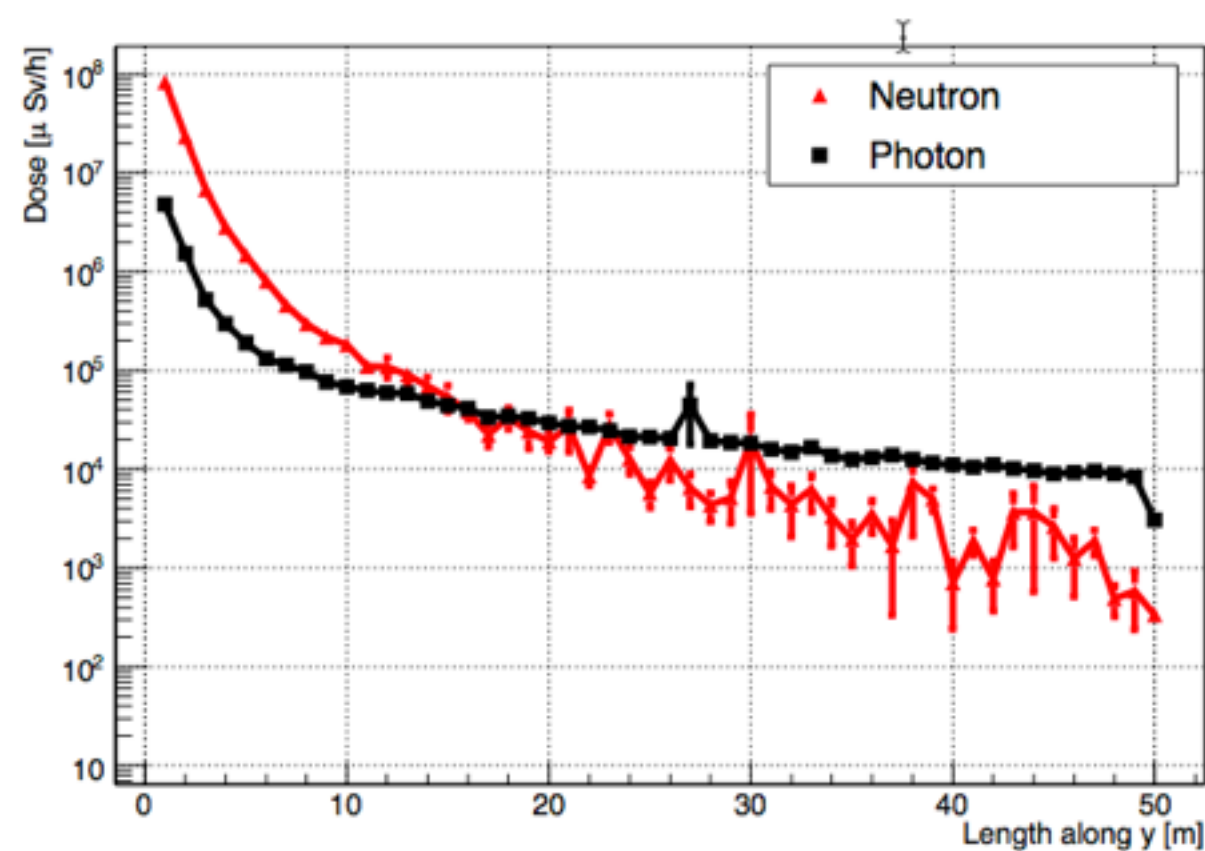
$$\mathbf{n}_r = (\mathbf{r}_r, \mathbf{v}_r, t_r, \mathbf{s}_r, p_r)$$

$$\mathbf{n}_i = (\mathbf{r}_i, \mathbf{v}_i, t_i, \mathbf{s}_i, p_i)$$

MCNPX



McStas



Collaboration
DTU Nutech
DTU Fysik
ESS

McStas-MCNPX interfaces for beam losses

1 m

1 m

5 cm

$$\mathbf{n}_t = (\mathbf{r}_t, \mathbf{v}_t, t_t, \mathbf{s}_t, p_i - p_r)$$

$$\mathbf{n}_r = (\mathbf{r}_r, \mathbf{v}_r, t_r, \mathbf{s}_r, p_r)$$

$$\mathbf{n}_i = (\mathbf{r}_i, \mathbf{v}_i, t_i, \mathbf{s}_i, p_i)$$

MCNPX

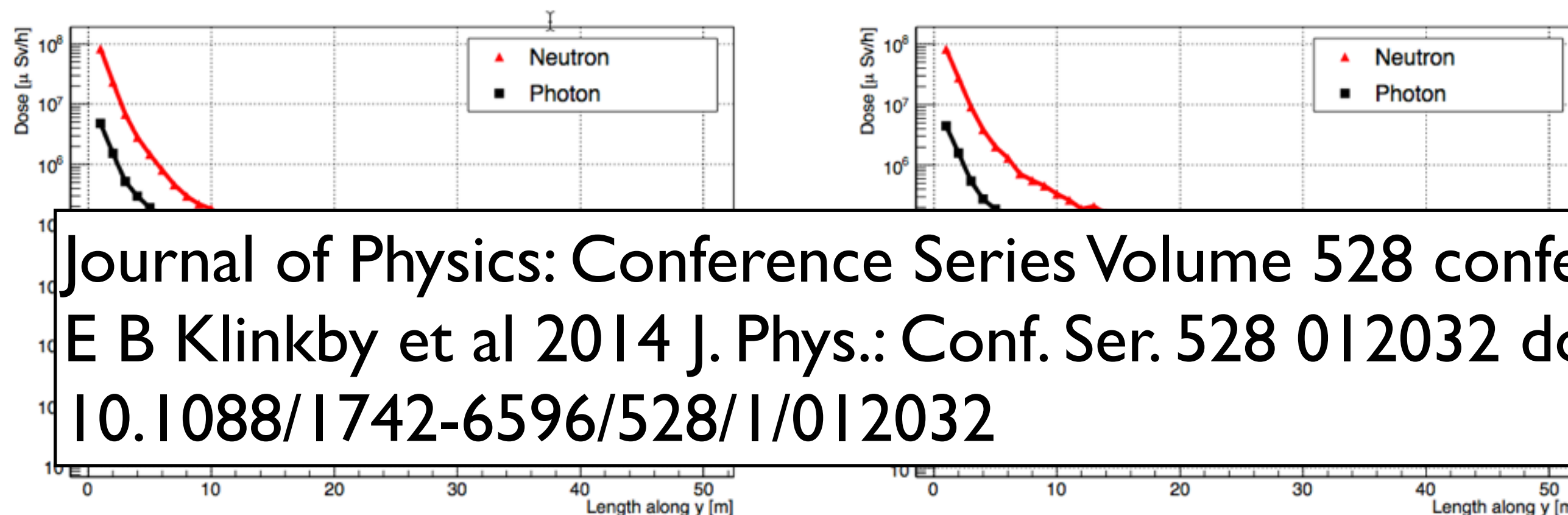


McStas



Use: Check the Scatter_logger.comp
in the McStas distribution

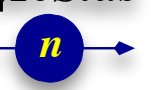
Future:
Geant4,
PHITS?



Collaboration
Nutech
Fysik

Journal of Physics: Conference Series Volume 528 conference I
E B Klinkby et al 2014 J. Phys.: Conf. Ser. 528 012032 doi:
10.1088/1742-6596/528/1/012032

McStas



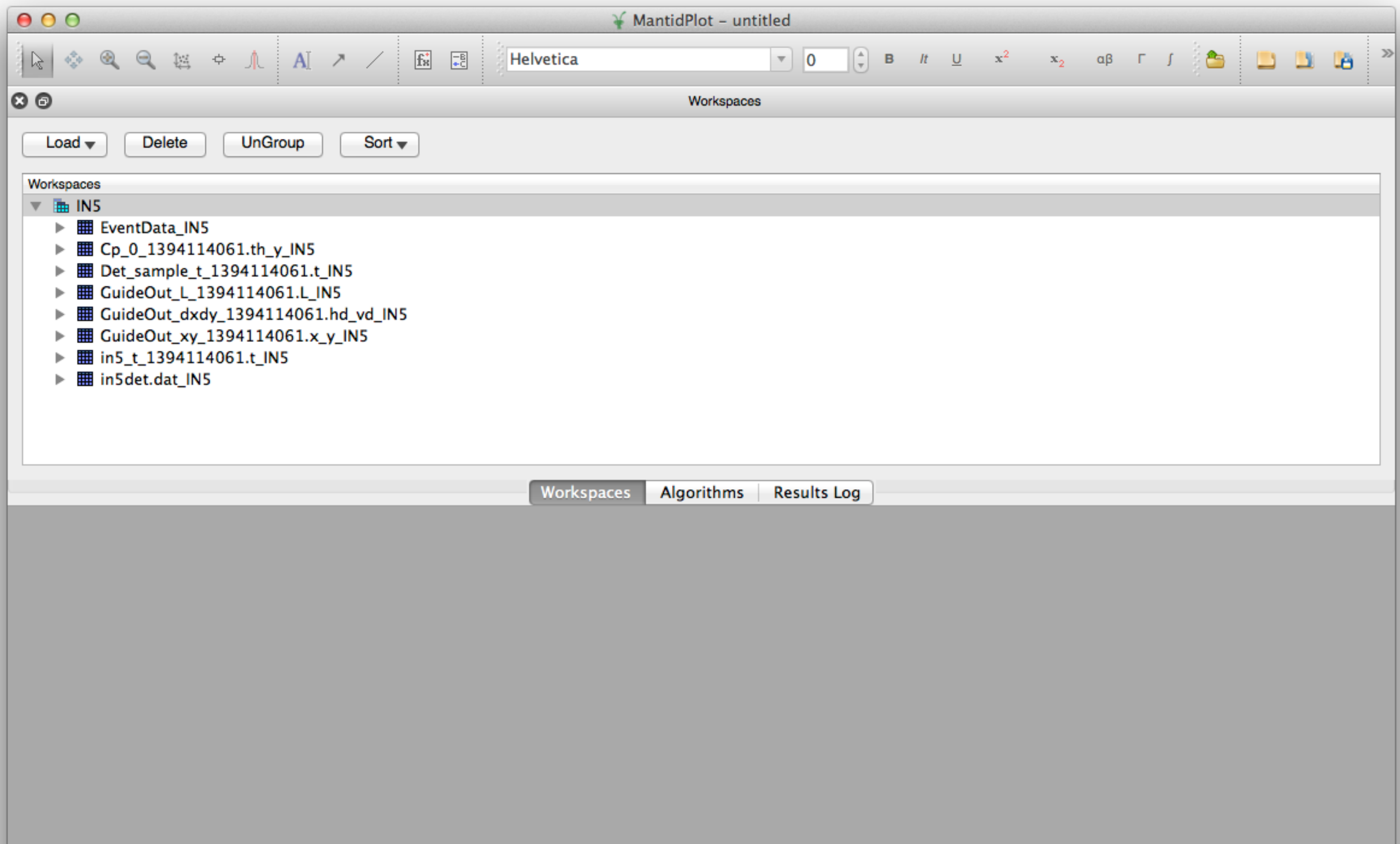
McStas-Mantid event processing facilitated by:

Special labels in component list

Special Monitor_nD paramers

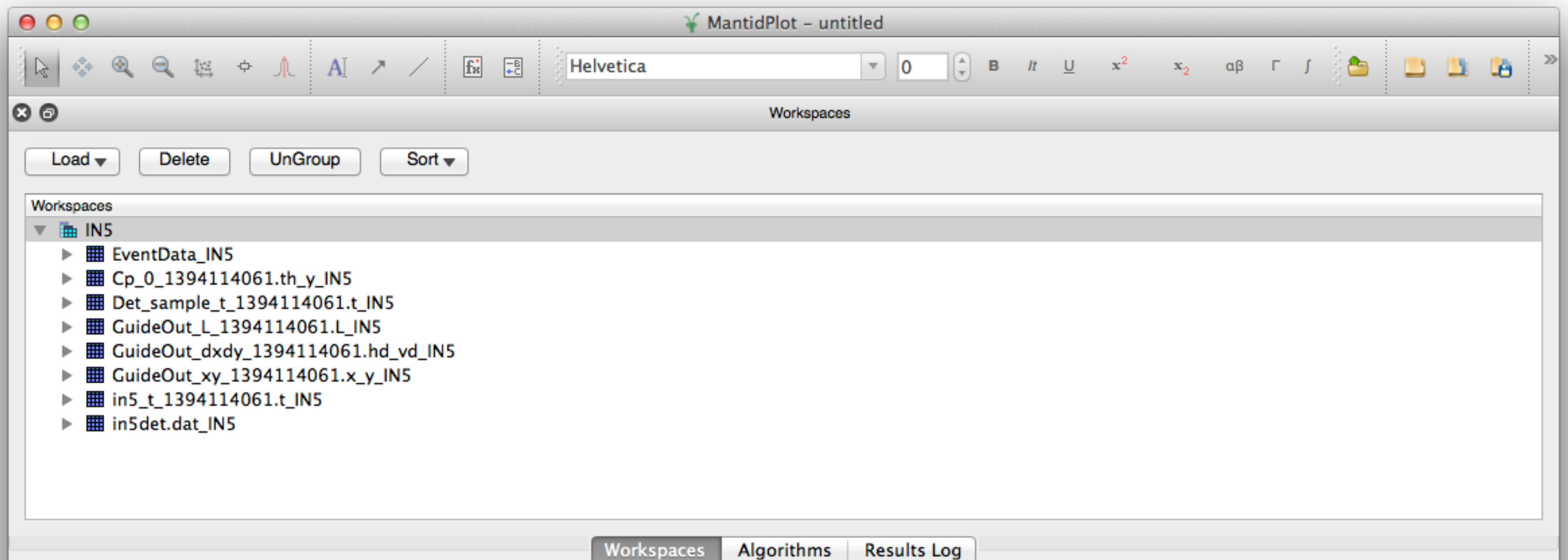
IDF autogenerated by “mcdisplay” run

NeXus output and LoadMcStas Mantid algorithm



McStas-Mantid event processing facilitated by:

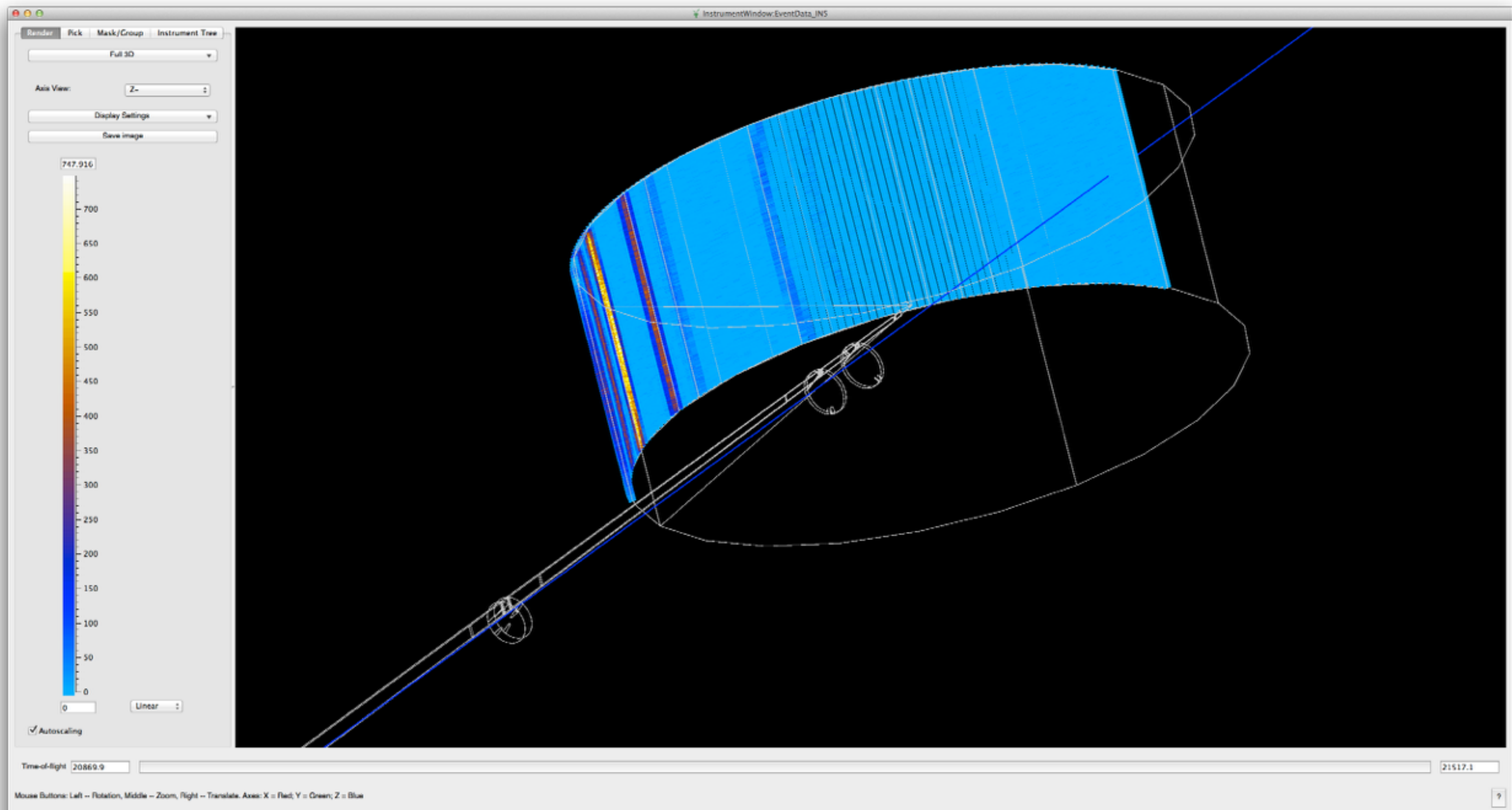
Special labels in component list
Special Monitor_nD paramers
IDF autogenerated by “mcdisplay” run
NeXus output and LoadMcStas Mantid algorithm



Use: Check out
templateSANS_Mantid
from the McStas distribution
- fully functional reduction

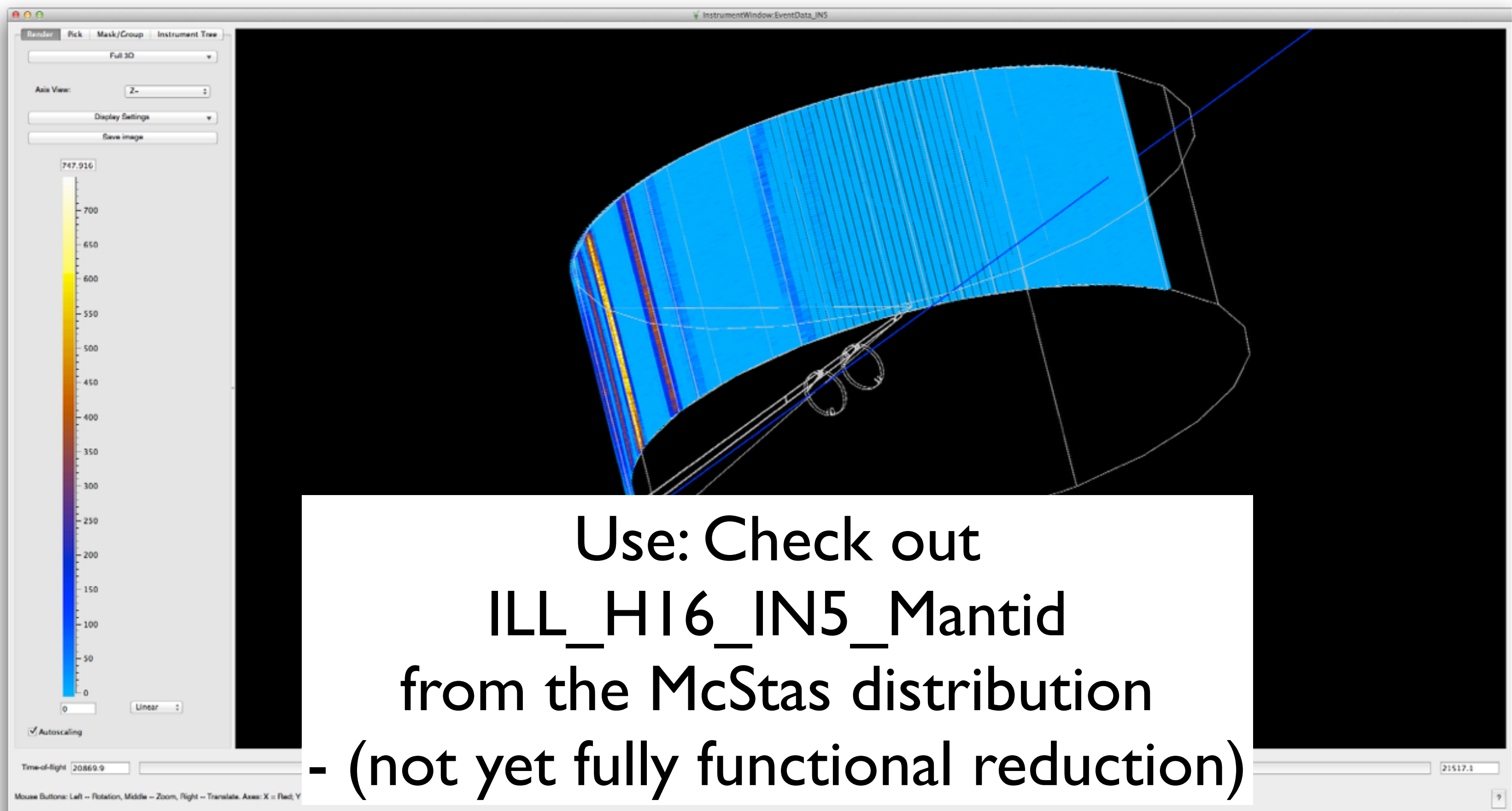
Events shown on the full instrument

- The event data from McStas should look something like this in “full 3D” - you may have to move/zoom a bit about



Events shown on the full instrument

- The event data from McStas should look something like this in “full 3D” - you may have to move/zoom a bit about



Problem: McStas Single_crystal.comp “slow” for large unit cell diffraction studies

- Example: Rubredoxin

Rubredoxin

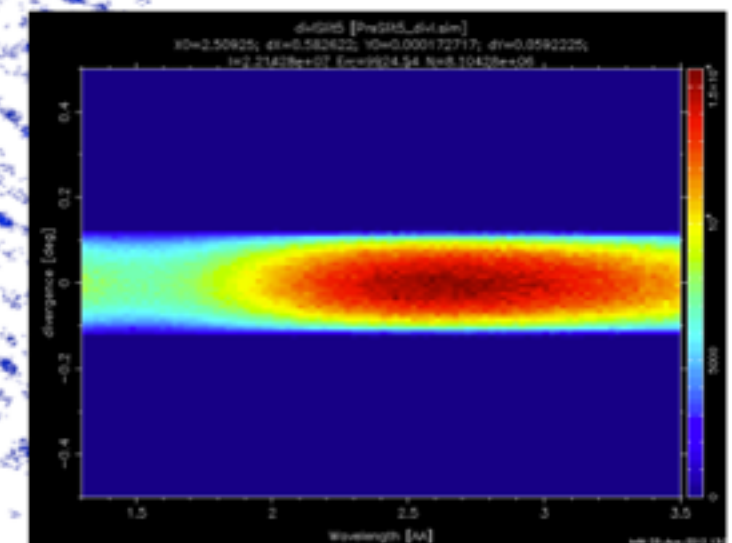
Images created from simulated datafile produced
August 20th 2012 using 25 nodes on the DMSC
cluster.

Neutron count: 1e12

Simulation time: ~10 + ~20 hr = ~30 hrs total

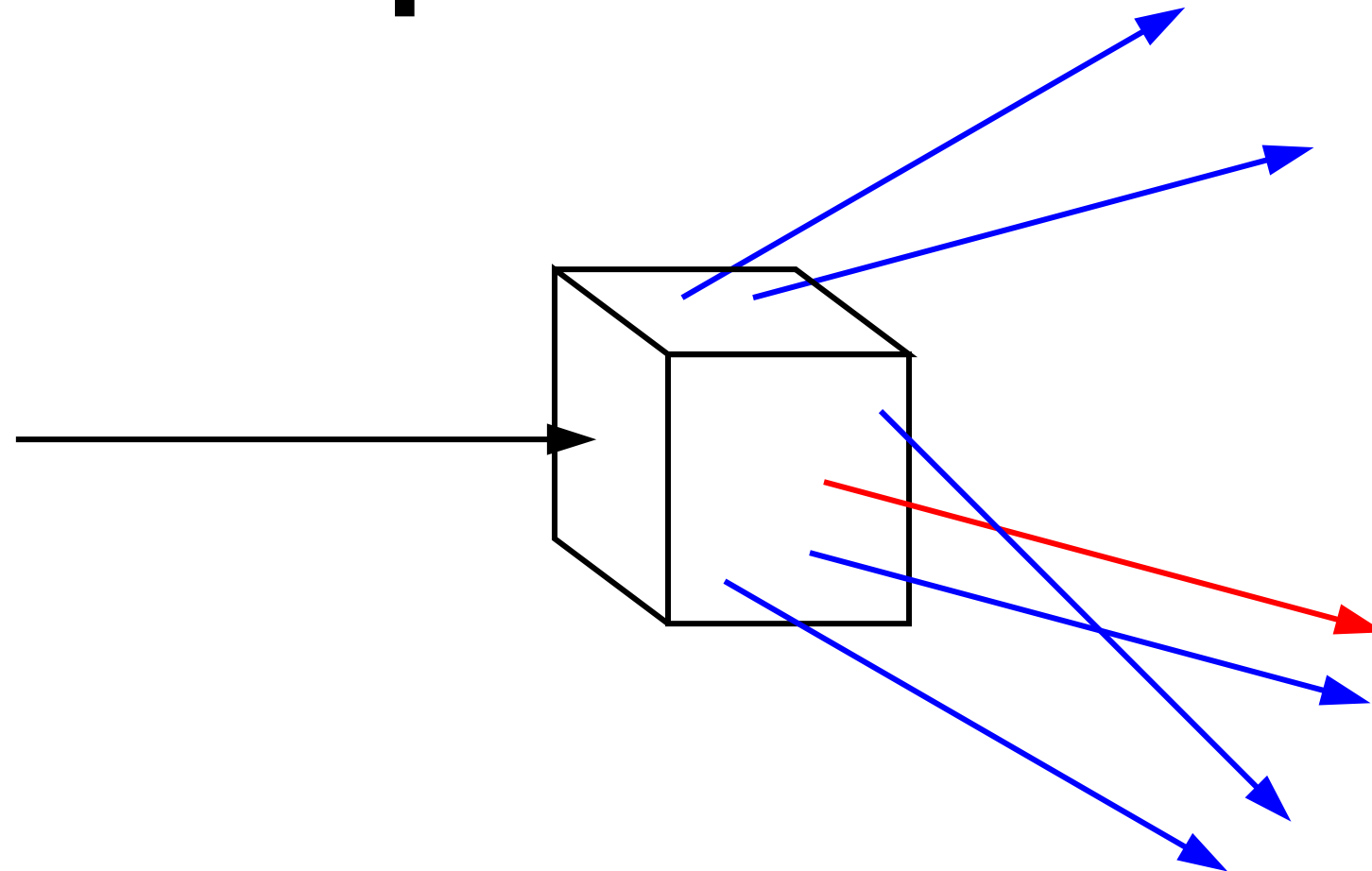
1 timebin, 1000 x,y-bins

Neutroncount: 1e12
No gravitation
Xtal size: 0.5 mm
Xtal mosaicity: 12'
Detector: 50 x 50 cm flat
Detector-to-sample
distance: 20 cm
Guide length: 131 m
Guide dimensions: 9.5 cm
 $\lambda_{\min} = 1.3 \text{ \AA}$
 $\lambda_{\max} = 3.5 \text{ \AA}$
Timespan: 51.39 to 143.4 ms
Divergence = 0.2 degs



- Reflection list ~ 124 K reflections (still “small” in the PX world!!)

Algorithm improvement: **Use incoming neutrons more efficiently - scatter each one on all possible reflections**

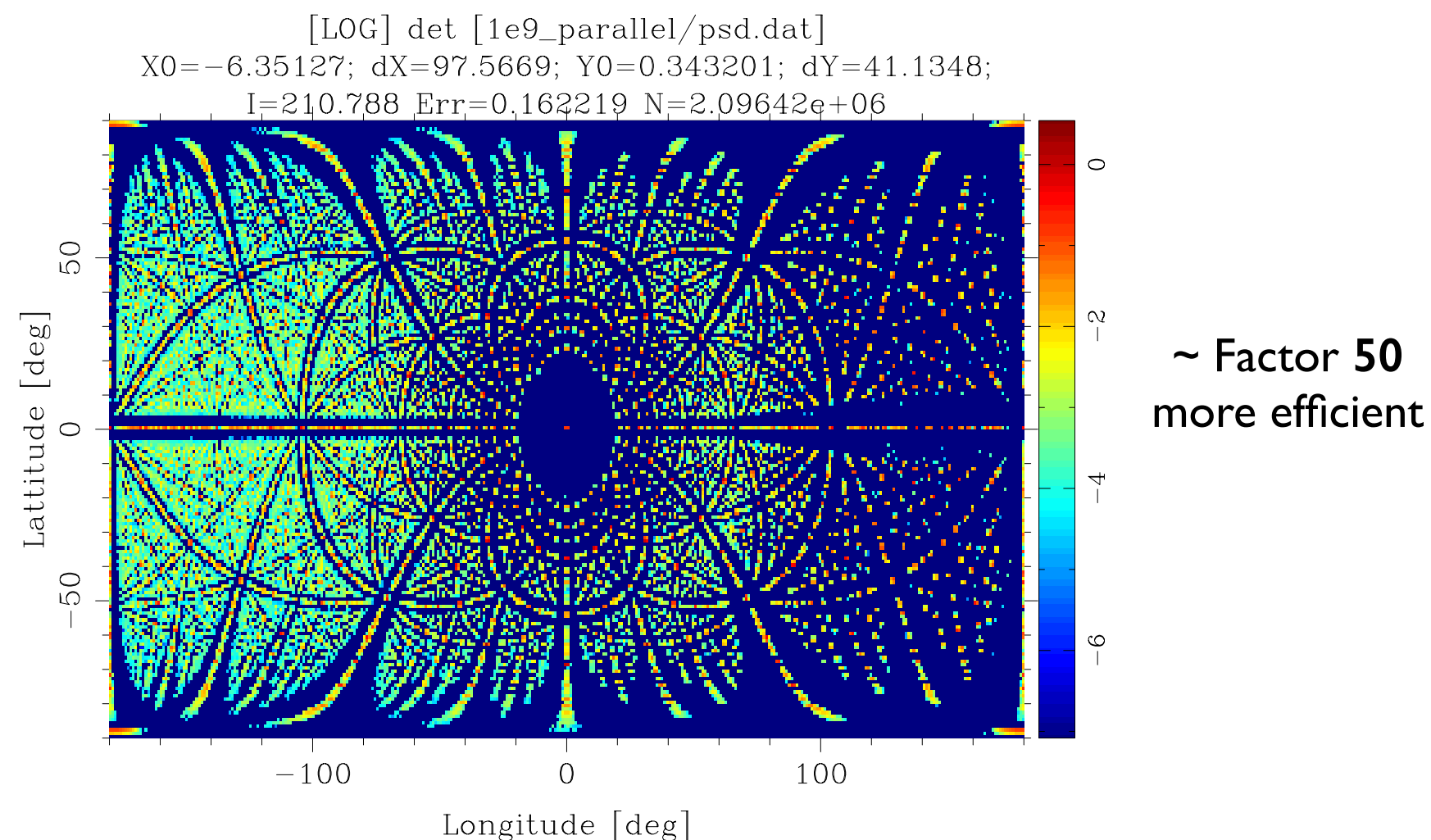
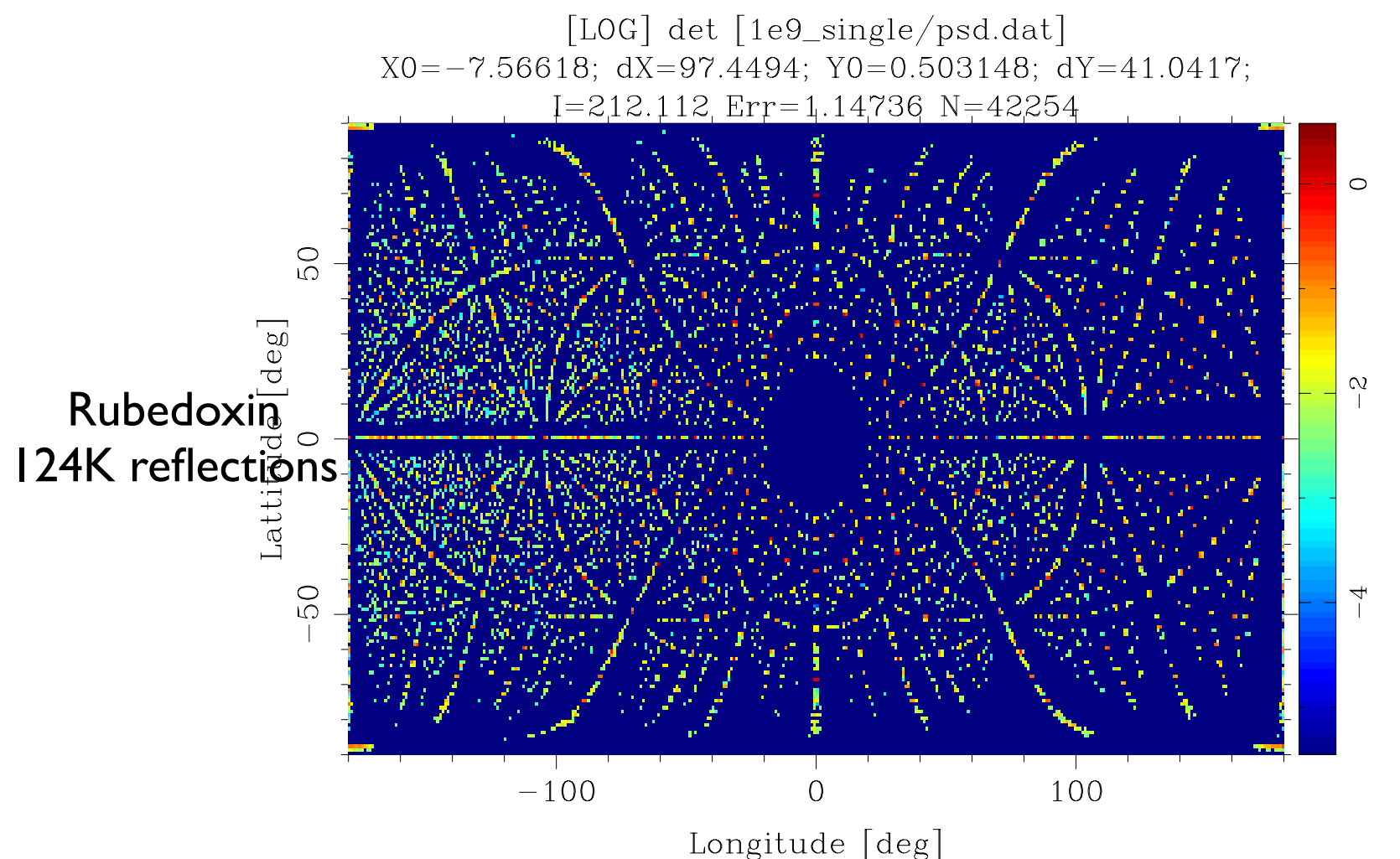


- **Red**: Original algorithm, one incoming neutron used only once
- **Blue**: Improved algorithm, each incoming neutron scattered (via SPLIT keyword) all possible times
- Component makes **estimate on average number of “active”** diffraction **spots** - in the case Rubredoxin this is around **50!**

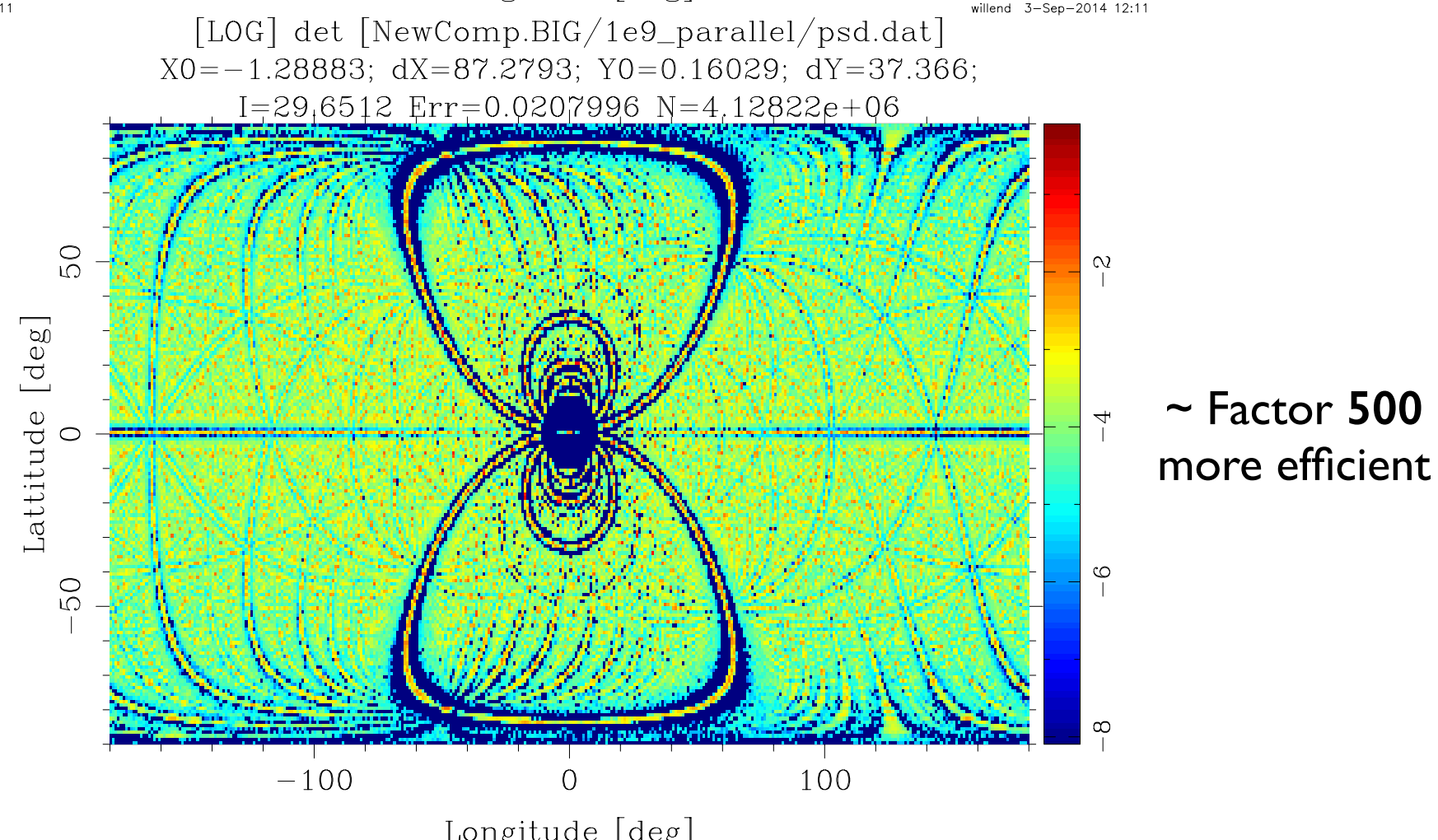
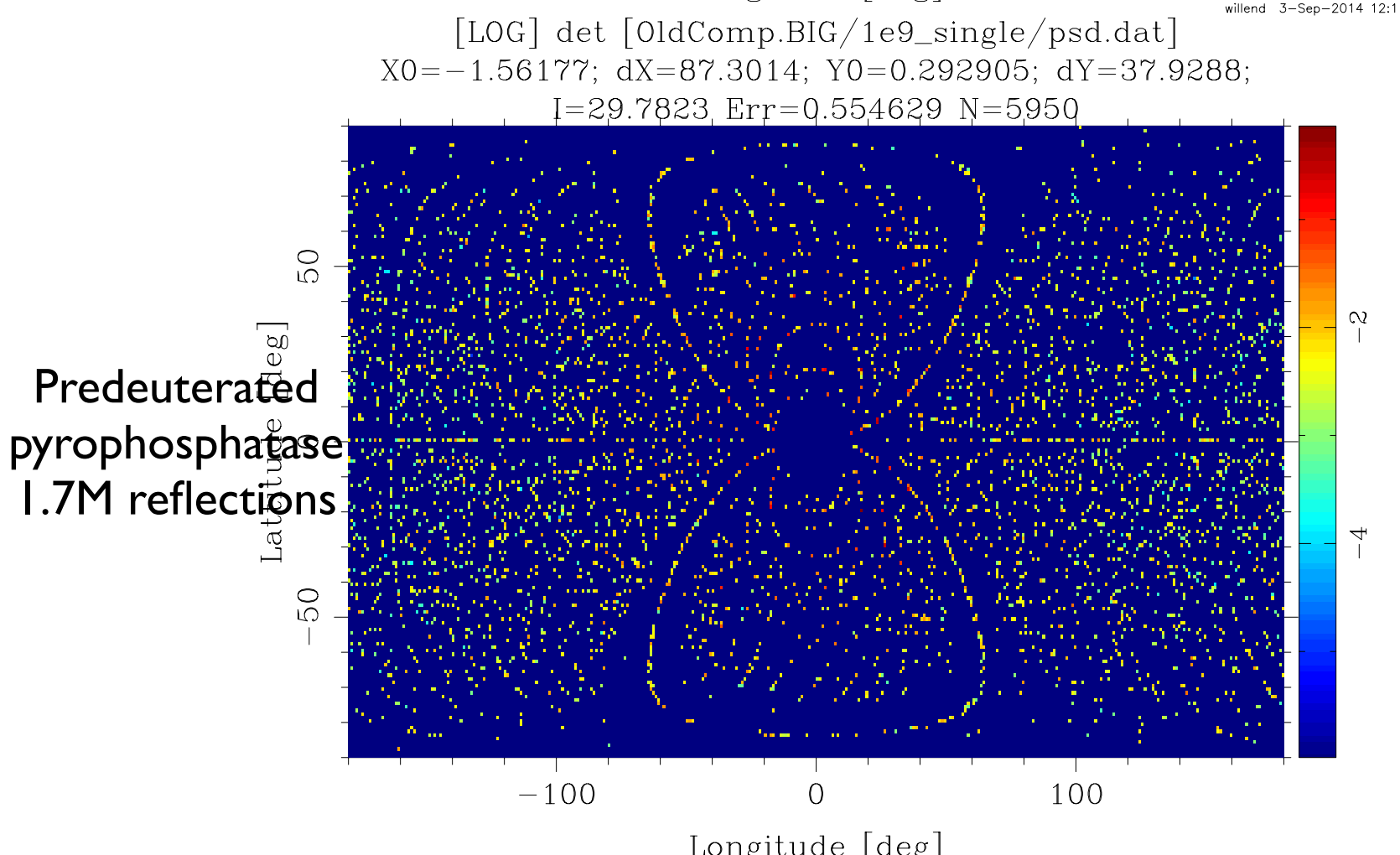
Sim data speak for themselves - 1e9 rays

Old comp

New comp



~ Factor 50
more efficient

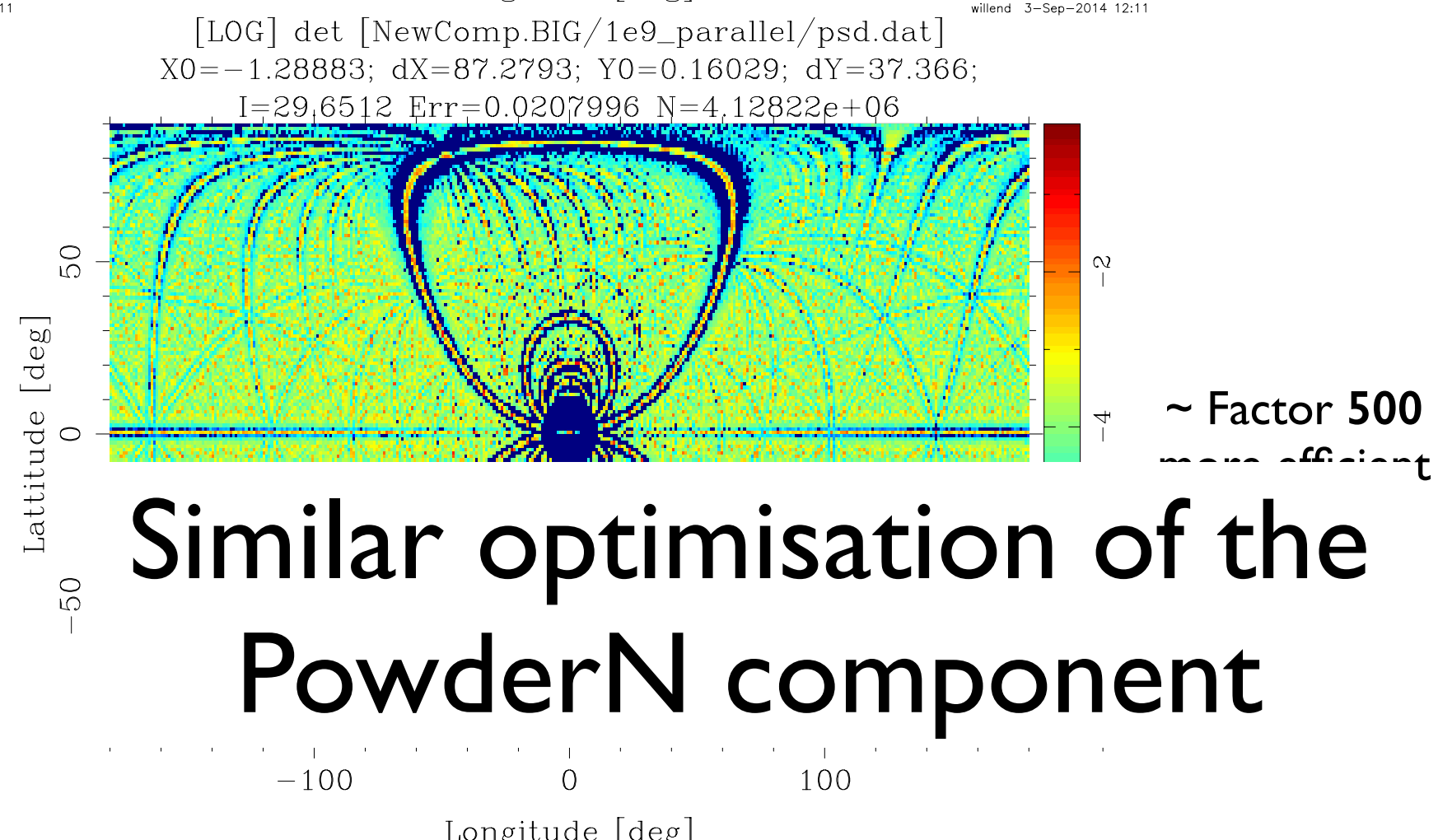
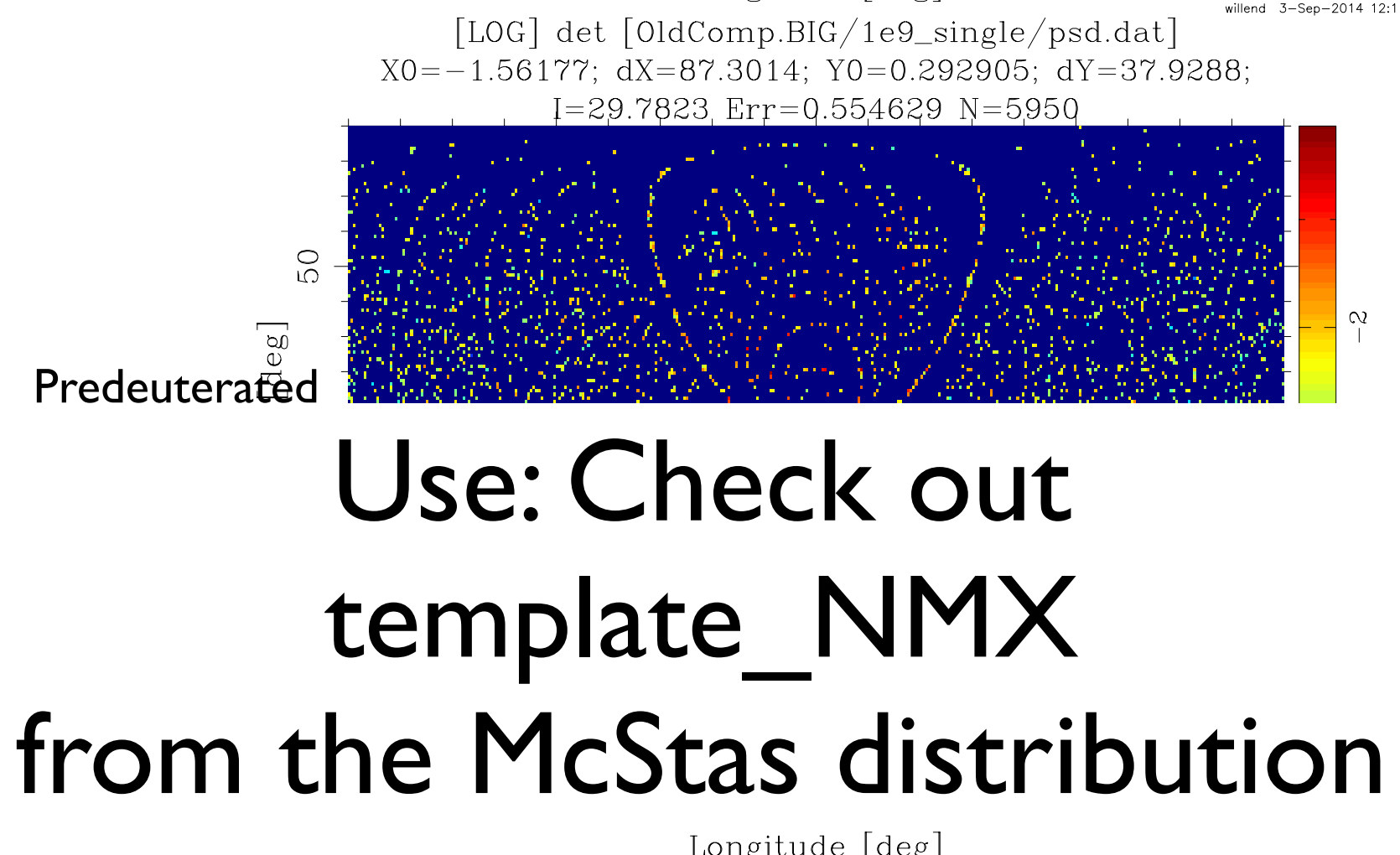
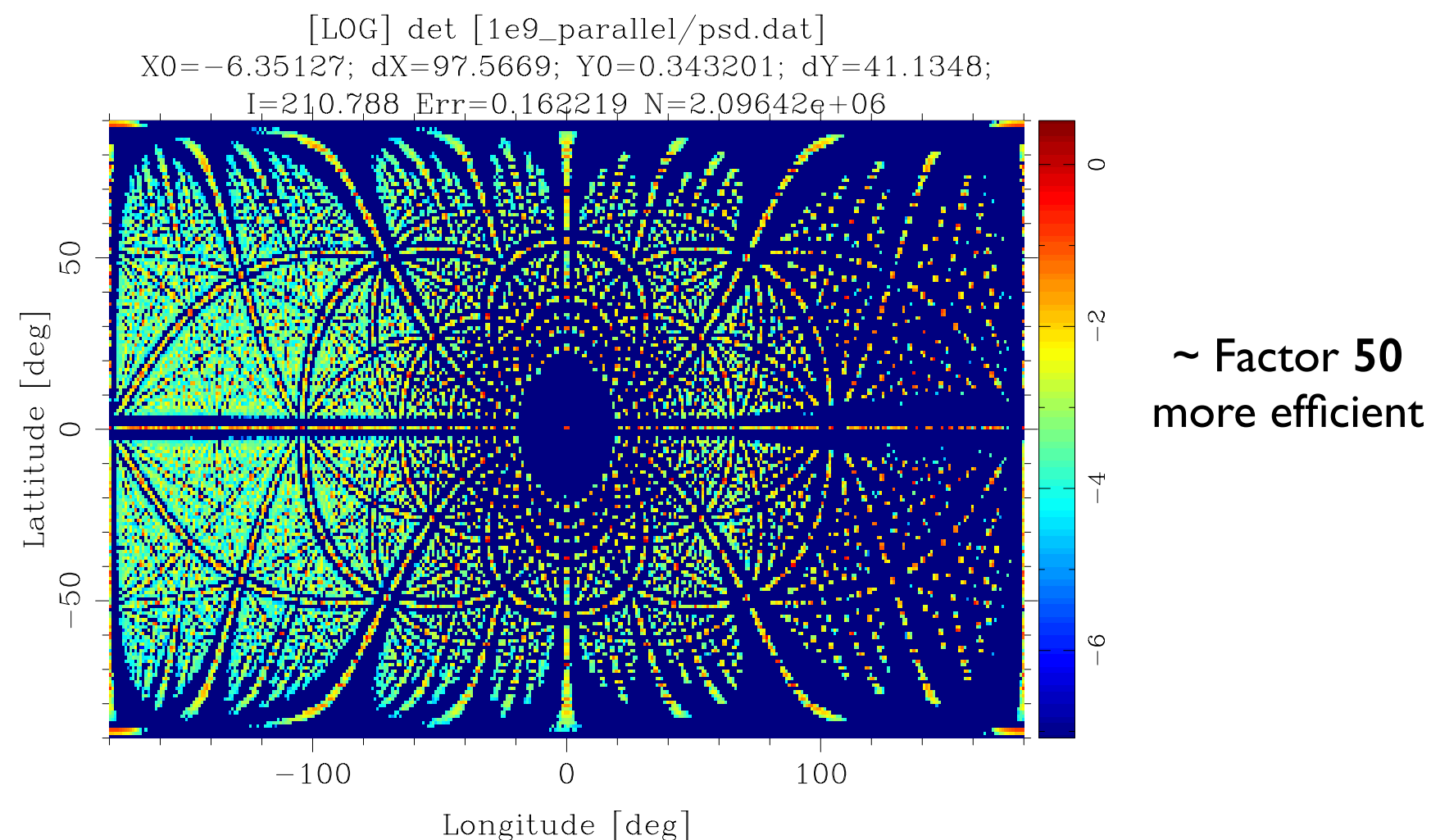
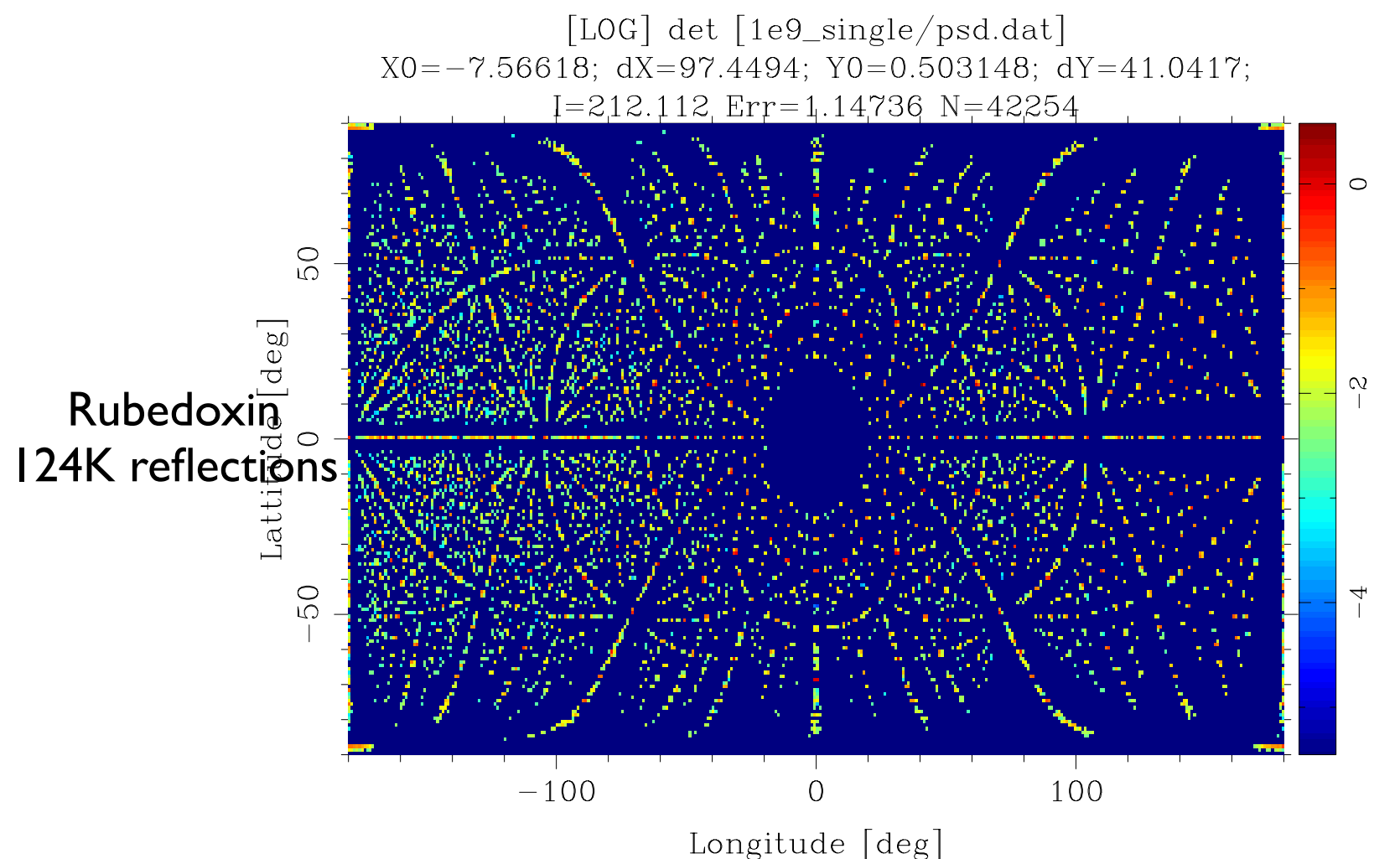


~ Factor 500
more efficient

Sim data speak for themselves - 1e9 rays

Old comp

New comp



Use: Check out
template_NMX
from the McStas distribution

Similar optimisation of the
PowderN component

People

- The success of the project is also about the people:
- Present McStas team members



• K Lefmann



E Farhi



P Willendrup



E Knudsen

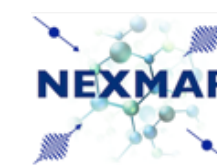
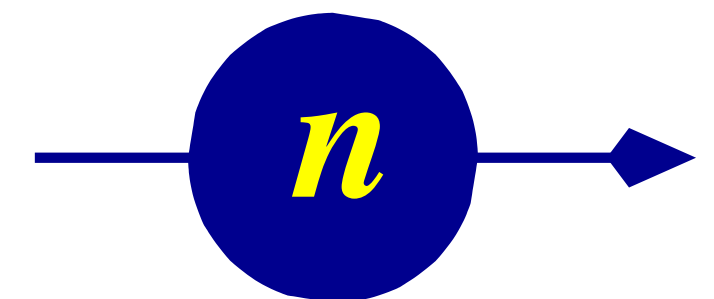


U Filges



T R Nielsen

McStas



- Past McStas team members



• K Nielsen



PO Åstrand



K Lieutenant



P Christiansen



J Brinch

New developments in McStas